STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 176380

TO: Marcela Cordero Garcia
Location: rem/3C35/3C18
Art Unit: 1654
Friday, January 20, 2006
Case Serial Number: 10/822639

From: John DiNatale
Location: Biotech-Chem Library
REM-1B65
Phone: (571)272-2557

john.dinatale@uspto.gov

Search Notes

Examiner Cordero Garcia,

See attached results.

If you have any questions about this search feel free to contact me at any time.

Thank you for using STIC search services!

John DiNatale
Technical Information Specialist
STIC Biotech/Chem Library
(571)272-2557

FOR OFFICIAL USE ONLY

ACCESS DB # 176380

PLEASE PRINT CLEARLY

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: MARCELA M CORDERO GARCIA Examiner # : 80381 Date: 1/11/06

Art Unit: 1654 Phone Number: 2-2939 Serial Number: 10/822,639

Location (Bldg/Room#): REM3C35 (Mailbox #): 3C18 Results Format Preferred (circle): PAPER DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following: MG

Title of Invention: MIXTURES OF ISOBARICALLY LABELED ANALYTES AND...

Inventors (please provide full names): (SEE ATTACHD BIB DS)

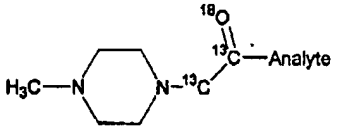
Earliest Priority Date: 1/5/04

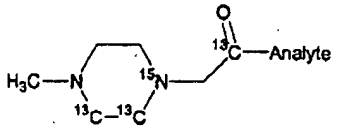
Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

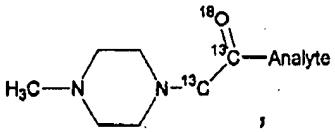
PLEASE SEARCH A MIXTURE OF THE COMPOUNDS:



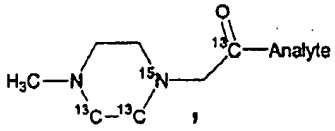


, WHEREIN ANALYTE = PEPTIDE / PROTEIN

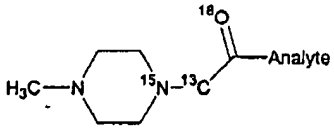
IF ONLY APPLICANT'S OWN WORK FOUND, PLEASE BROADEN SEARCH TO ENCOMPASS AT LEAST TWO OF THE FOLLOWING COMPOUNDS:



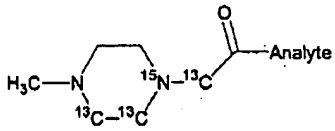
,



,



and



, WHEREIN ANALYTE = OPEN (ANY MOLECULE) OR ATOMS

THANKS,

****

STAFF USE ONLY

Searcher: _____

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: 1/20/06

Searcher Prep & Review Time: _____

Online Time: _____

Type of Search

_____ NA Sequence (#)

_____ AA Sequence (#)

_____ Structure (#)

_____ Bibliographic

_____ Litigation

_____ Fulltext

_____ Other

Vendors and cost where applicable

_____ STN _____ Dialog

_____ Questel/Orbit _____ Lexis/Nexis

_____ Westlaw _____ WWW/Internet

____ In-house sequence systems

____ Commercial ____ Oligomer ____ Score/Length

____ Interference ____ SPDI ____ Encode/Transl

_____ Other (specify)

Search history

Cordero-Garcia 10/822639 01/20/2006

```
=> d his full

     (FILE 'HOME' ENTERED AT 10:13:10 ON 20 JAN 2006)

     FILE 'REGISTRY' ENTERED AT 10:13:24 ON 20 JAN 2006
L1             SCREEN 2039
L2             STRUCTURE UPLOADED
L3           1 SEA SSS SAM L1 AND L2
               D SCA
L4          81 SEA SSS FUL L1 AND L2

     FILE 'CAPLUS' ENTERED AT 10:14:39 ON 20 JAN 2006
L5          29 SEA ABB=ON  PLU=ON  L4

     FILE 'REGISTRY' ENTERED AT 10:16:14 ON 20 JAN 2006
L6             ANALYZE PLU=ON  L4 1- LC :       5 TERMS
               D

     FILE 'USPATFULL' ENTERED AT 10:17:51 ON 20 JAN 2006
L7          13 SEA ABB=ON  PLU=ON  L4

     FILE 'CAPLUS, USPATFULL' ENTERED AT 10:18:30 ON 20 JAN 2006
L8          36 DUP REM L5 L7 (6 DUPLICATES REMOVED)
                   ANSWERS '1-29' FROM FILE CAPLUS
                   ANSWERS '30-36' FROM FILE USPATFULL

     FILE 'CHEMCATS' ENTERED AT 10:18:50 ON 20 JAN 2006
L9           1 SEA ABB=ON  PLU=ON  L4

     FILE 'REGISTRY' ENTERED AT 10:19:20 ON 20 JAN 2006

     FILE 'CAPLUS' ENTERED AT 10:21:20 ON 20 JAN 2006
               E PAPPIN/AU
L10        109 SEA ABB=ON  PLU=ON  PAPPIN D?/AU
               E PURKAY/AU
L11         45 SEA ABB=ON  PLU=ON  PURKAYASTHA S?/AU
L12        168 SEA ABB=ON  PLU=ON  COULL J?/AU
L13          5 SEA ABB=ON  PLU=ON  L10 AND L11 AND L12
L14         14 SEA ABB=ON  PLU=ON  (L10 AND (L11 OR L12)) OR (L11 AND L12)
L15          8 SEA ABB=ON  PLU=ON  (L10 OR L11 OR L12) AND L5

     FILE 'USPATFULL' ENTERED AT 10:24:48 ON 20 JAN 2006
L16         16 SEA ABB=ON  PLU=ON  PAPPIN D?/AU
L17          7 SEA ABB=ON  PLU=ON  PURKAYASTHA S?/AU
L18         46 SEA ABB=ON  PLU=ON  COULL J?/AU
L19          5 SEA ABB=ON  PLU=ON  L16 AND L17 AND L18
L20          8 SEA ABB=ON  PLU=ON  (L16 AND (L17 OR L18)) OR (L17 AND L18)
L21         10 SEA ABB=ON  PLU=ON  L7 AND (L16 OR L17 OR L18)

     FILE 'REGISTRY' ENTERED AT 10:27:44 ON 20 JAN 2006
L*** DEL      9 S L4 AND CASREACT/LC NOT CAPLUS/LS
L22           0 SEA ABB=ON  PLU=ON  L4 AND CASREACT/LC NOT CAPLUS/LC

     FILE 'REGISTRY' ENTERED AT 10:29:02 ON 20 JAN 2006
               D STAT QUE L4
               D L6
               D QUE L22

     FILE 'REGISTRY' ENTERED AT 10:30:44 ON 20 JAN 2006
```

```
                D STAT QUE L4
                D L6
                D QUE NOS L22

     FILE 'CASREACT' ENTERED AT 10:31:49 ON 20 JAN 2006
L23           6 SEA ABB=ON  PLU=ON  L4

     FILE 'CAPLUS, CASREACT' ENTERED AT 10:32:22 ON 20 JAN 2006
L24          29 DUP REM L5 L23 (6 DUPLICATES REMOVED)
                    ANSWERS '1-29' FROM FILE CAPLUS

     FILE 'REGISTRY' ENTERED AT 10:32:44 ON 20 JAN 2006

     FILE 'REGISTRY' ENTERED AT 10:33:02 ON 20 JAN 2006
                D STAT QUE L4
                D L6

     FILE 'CAPLUS' ENTERED AT 10:36:02 ON 20 JAN 2006
                D QUE L13
                D QUE NOS L14
                D QUE NOS L15
L25          16 SEA ABB=ON  PLU=ON  L13 OR L14 OR L15

     FILE 'USPATFULL' ENTERED AT 10:37:09 ON 20 JAN 2006
                D QUE L19
                D QUE NOS L20
                D QUE NOS L21
L26          12 SEA ABB=ON  PLU=ON  L19 OR L20 OR L21

     FILE 'CAPLUS, USPATFULL' ENTERED AT 10:38:26 ON 20 JAN 2006
L27          22 DUP REM L25 L26 (6 DUPLICATES REMOVED)
                    ANSWERS '1-16' FROM FILE CAPLUS
                    ANSWERS '17-22' FROM FILE USPATFULL
                D IBIB ABS HITIND HITSTR L27 1-16
                D IBIB ABS HITSTR L27 17-22

     FILE 'CAPLUS' ENTERED AT 10:42:08 ON 20 JAN 2006
                D QUE L5

     FILE 'CAPLUS' ENTERED AT 10:42:42 ON 20 JAN 2006
                D QUE NOS L5
L28          21 SEA ABB=ON  PLU=ON  L5 NOT L25

     FILE 'CASREACT' ENTERED AT 10:44:21 ON 20 JAN 2006
                D QUE NOS L23

     FILE 'USPATFULL' ENTERED AT 10:44:50 ON 20 JAN 2006
                D QUE NOS L7
L29           3 SEA ABB=ON  PLU=ON  L7 NOT L26

     FILE 'CHEMCATS' ENTERED AT 10:45:20 ON 20 JAN 2006
                D QUE NOS L9

     FILE 'CAPLUS, CASREACT, USPATFULL, CHEMCATS' ENTERED AT 10:46:16 ON 20
     JAN 2006
L30          25 DUP REM L28 L23 L29 L9 (6 DUPLICATES REMOVED)
                    ANSWERS '1-21' FROM FILE CAPLUS
                    ANSWERS '22-24' FROM FILE USPATFULL
                    ANSWER '25' FROM FILE CHEMCATS
```

```
          D IBIB ABS HITIND HITSTR L30 1-21
          D IBIB ABS HITSTR L30 22-24
          D IALL L30 25

FILE 'STNGUIDE' ENTERED AT 10:50:09 ON 20 JAN 2006


FILE HOME

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   18 JAN 2006  HIGHEST RN 872163-75-2
DICTIONARY FILE UPDATES:  18 JAN 2006  HIGHEST RN 872163-75-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*************************************************************
*                                                           *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                           *
*************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE CAPLUS

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
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FILE COVERS 1907 - 20 Jan 2006  VOL 144 ISS 5
FILE LAST UPDATED: 19 Jan 2006  (20060119/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:
```

http://www.cas.org/infopolicy.html

FILE USPATFULL
FILE COVERS 1971 TO PATENT PUBLICATION DATE: 19 Jan 2006 (20060119/PD)
FILE LAST UPDATED: 19 Jan 2006 (20060119/ED)
HIGHEST GRANTED PATENT NUMBER: US6988280
HIGHEST APPLICATION PUBLICATION NUMBER: US2006015978
CA INDEXING IS CURRENT THROUGH 19 Jan 2006 (20060119/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 19 Jan 2006 (20060119/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2005

FILE CHEMCATS

FILE LAST UPDATED 14 JANUARY 2006 (20060114/UP)

For details on recent updates in CHEMCATS, enter NEWS FILE at an arrow prompt. For the list of suppliers currently in the file, enter HELP SPA, HELP SPBC, HELP SPDH, HELP SPIN, HELP SPOP, and HELP SPQZ. For the list of current catalogs, enter HELP CTA, HELP CTBC, HELP CTDH, HELP CTIN, HELP CTOP, and HELP CTQZ.

This database is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this database.

CHEMCATS now contains more than 8 million records. See HELP CONTENT and NEWS FILE for details.

FILE CASREACT
Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 15 Jan 2006 VOL 144 ISS 3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
**********************************************************
*                                                        *
*     CASREACT now has more than 10 million reactions    *
*                                                        *
**********************************************************
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jan 13, 2006 (20060113/UP).

```
=> file registry
FILE 'REGISTRY' ENTERED AT 10:33:02 ON 20 JAN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   18 JAN 2006  HIGHEST RN 872163-75-2
DICTIONARY FILE UPDATES:  18 JAN 2006  HIGHEST RN 872163-75-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*************************************************************************
*                                                                       *
* The CA roles and document type information have been removed from     *
* the IDE default display format and the ED field has been added,       *
* effective March 20, 2005.  A new display format, IDERL, is now        *
* available and contains the CA role and document type information.     *
*                                                                       *
*************************************************************************

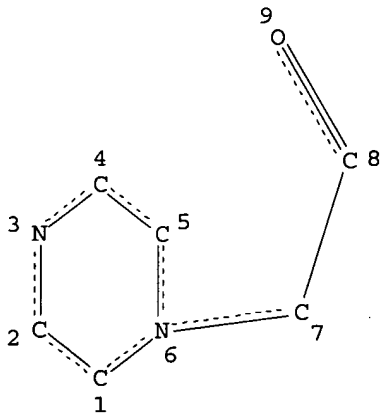
Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d stat que L4
L1              SCR 2039
L2              STR
```

← Screen for abnormal mass (e.g. isotopically labeled)



NODE ATTRIBUTES:

```
NSPEC   IS R      AT   1
NSPEC   IS R      AT   2
NSPEC   IS R      AT   3
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS C      AT   7
NSPEC   IS C      AT   8
NSPEC   IS C      AT   9
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   7  8  9
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
L4            81 SEA FILE=REGISTRY SSS FUL L1 AND L2

100.0% PROCESSED     814 ITERATIONS                    81 ANSWERS
SEARCH TIME: 00.00.01


=> d L6
L6          ANALYZE L4 1- LC :       5 TERMS

TERM #   # OCC  # DOC  % DOC LC
------ ------- ------ ------ ---------------
     1      66     66  81.48 CA
     2      66     66  81.48 CAPLUS
     3      41     41  50.62 USPATFULL
     4       9      9  11.11 CASREACT
     5       1      1   1.23 CHEMCATS
*********  END OF L6 ***
```

81 structures

4 database locations

```
=> file caplus
FILE 'CAPLUS' ENTERED AT 10:36:02 ON 20 JAN 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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```

AUTHOR SEARCH


```
FILE COVERS 1907 - 20 Jan 2006  VOL 144 ISS 5
FILE LAST UPDATED: 19 Jan 2006  (20060119/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
```

They are available for your review at:

http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

```
=> d que L13
L10          109 SEA FILE=CAPLUS ABB=ON  PLU=ON  PAPPIN D?/AU
L11           45 SEA FILE=CAPLUS ABB=ON  PLU=ON  PURKAYASTHA S?/AU
L12          168 SEA FILE=CAPLUS ABB=ON  PLU=ON  COULL J?/AU
L13            5 SEA FILE=CAPLUS ABB=ON  PLU=ON  L10 AND L11 AND L12

=> d que nos L14
L10          109 SEA FILE=CAPLUS ABB=ON  PLU=ON  PAPPIN D?/AU
L11           45 SEA FILE=CAPLUS ABB=ON  PLU=ON  PURKAYASTHA S?/AU
L12          168 SEA FILE=CAPLUS ABB=ON  PLU=ON  COULL J?/AU
L14           14 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L10 AND (L11 OR L12)) OR (L11
                 AND L12)

=> d que nos L15
L1               SCR 2039
L2               STR
L4            81 SEA FILE=REGISTRY SSS FUL L1 AND L2
L5            29 SEA FILE=CAPLUS ABB=ON  PLU=ON  L4
L10          109 SEA FILE=CAPLUS ABB=ON  PLU=ON  PAPPIN D?/AU
L11           45 SEA FILE=CAPLUS ABB=ON  PLU=ON  PURKAYASTHA S?/AU
L12          168 SEA FILE=CAPLUS ABB=ON  PLU=ON  COULL J?/AU
L15            8 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L10 OR L11 OR L12) AND L5

=> s L13 or L14 or L15
L25           16 L13 OR L14 OR L15

=> file uspatfull
FILE 'USPATFULL' ENTERED AT 10:37:09 ON 20 JAN 2006
CA INDEXING COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 19 Jan 2006 (20060119/PD)
FILE LAST UPDATED: 19 Jan 2006 (20060119/ED)
HIGHEST GRANTED PATENT NUMBER: US6988280
HIGHEST APPLICATION PUBLICATION NUMBER: US2006015978
CA INDEXING IS CURRENT THROUGH 19 Jan 2006 (20060119/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 19 Jan 2006 (20060119/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2005

=> d que L19
L16           16 SEA FILE=USPATFULL ABB=ON  PLU=ON  PAPPIN D?/AU
L17            7 SEA FILE=USPATFULL ABB=ON  PLU=ON  PURKAYASTHA S?/AU
L18           46 SEA FILE=USPATFULL ABB=ON  PLU=ON  COULL J?/AU
L19            5 SEA FILE=USPATFULL ABB=ON  PLU=ON  L16 AND L17 AND L18

=> d que nos L20
L16           16 SEA FILE=USPATFULL ABB=ON  PLU=ON  PAPPIN D?/AU
L17            7 SEA FILE=USPATFULL ABB=ON  PLU=ON  PURKAYASTHA S?/AU
L18           46 SEA FILE=USPATFULL ABB=ON  PLU=ON  COULL J?/AU
```

```
L20             8 SEA FILE=USPATFULL ABB=ON  PLU=ON  (L16 AND (L17 OR L18)) OR
                  (L17 AND L18)


=> d que nos L21
L1                SCR 2039
L2                STR
L4               81 SEA FILE=REGISTRY SSS FUL L1 AND L2
L7               13 SEA FILE=USPATFULL ABB=ON  PLU=ON  L4
L16              16 SEA FILE=USPATFULL ABB=ON  PLU=ON  PAPPIN D?/AU
L17               7 SEA FILE=USPATFULL ABB=ON  PLU=ON  PURKAYASTHA S?/AU
L18              46 SEA FILE=USPATFULL ABB=ON  PLU=ON  COULL J?/AU
L21              10 SEA FILE=USPATFULL ABB=ON  PLU=ON  L7 AND (L16 OR L17 OR L18)


=> s L19 or L20 or L21
L26             12 L19 OR L20 OR L21

=> dup rem L25 L26
FILE 'CAPLUS' ENTERED AT 10:38:26 ON 20 JAN 2006
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FILE 'USPATFULL' ENTERED AT 10:38:26 ON 20 JAN 2006
CA INDEXING COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L25
PROCESSING COMPLETED FOR L26
L27             22 DUP REM L25 L26 (6 DUPLICATES REMOVED)
                   ANSWERS '1-16' FROM FILE CAPLUS
                   ANSWERS '17-22' FROM FILE USPATFULL

=> d ibib abs hitind hitstr L27 1-16; d ibib abs hitstr L27 17-22

L27  ANSWER 1 OF 22  CAPLUS  COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2005:588426  CAPLUS
DOCUMENT NUMBER:          143:115568
TITLE:                    Preparation of isotopically enriched N-substituted
                          piperazine-1-acetic acids
INVENTOR(S):              Dey, Subhakar; Pappin, Darryl J. c.;
                          Purkayastha, Subhasish; Pillai, Sasi;
                          Coull, James M.
PATENT ASSIGNEE(S):       Applera Corp., USA
SOURCE:                   U.S. Pat. Appl. Publ., 29 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   6
PATENT INFORMATION:

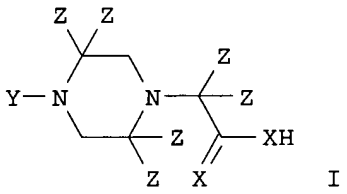
     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     US 2005148774         A1    20050707    US 2004-751387           20040105
     WO 2005068446         A1    20050728    WO 2005-US223            20050105
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
```

TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
US 2004-751353 A 20040105
US 2004-751354 A 20040105
US 2004-751387 A 20040105
US 2004-751388 A 20040105
US 2004-822639 A 20040412
US 2004-852730 A 20040524

OTHER SOURCE(S): MARPAT 143:115568

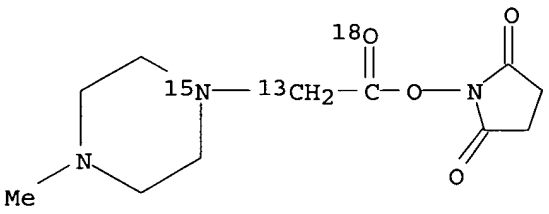
GI



I

AB Isotopically enriched N-substituted piperazine-1-acetic acids (I) or salts thereof, comprising one or more heavy atom isotopes [X = O, S; Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or F atoms; Z = independently H, deuterium, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms), a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms, or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms)] are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like. Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic

acid-1,2-13C.
IC ICM C07D241-04
INCL 544399000
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 6, 80
IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
IT 79-08-3DP, Bromoacetic acid, trityl chloride resin-bound 5672-86-6P, Trifluoroacetic acid pentachlorophenyl ester 5672-89-9P, Trifluoroacetic acid succinimidyl ester 54699-92-2P, 4-Methylpiperazine-1-acetic acid 145142-92-3P 145142-94-5P **856187-64-9P 856187-68-3P**
856187-72-9P 856187-80-9P **856187-83-2P**
856188-16-4P 856188-80-2P 856188-88-0P, Trifluoroacetic acid 2-oxopyrrolidin-1-yl ester **857027-04-4P 857027-05-5P**
857027-07-7P 857502-95-5P 857502-96-6P 857502-97-7P 857502-98-8P
857502-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
IT **856187-76-3P 856187-87-6P 856187-92-3P**
856188-02-8P, 4-Methylpiperazine-1-acetic acid 1,1,1,3,3,3-hexafluoropropan-2-yl ester 856188-06-2P 856188-23-3P 856188-27-7P
856188-32-4P 856188-37-9P 856188-38-0P 856188-43-7P 856188-44-8P
856188-49-3P 856188-50-6P 856188-62-0P **856290-53-4P**
856290-55-6P 857027-09-9P 857027-10-2P **857027-11-3P**
857027-12-4P 857503-00-5P 857503-01-6P 857503-02-7P
857503-03-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
RN 856188-20-0 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

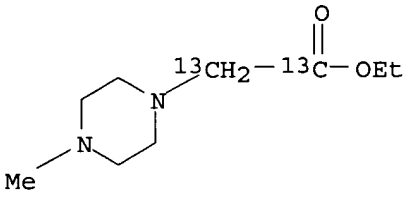


●2 HCl

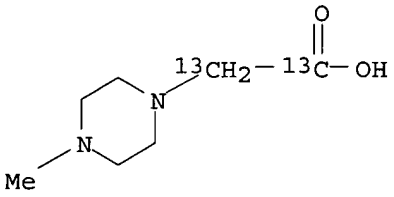
IT **856187-64-9P 856187-68-3P 856187-72-9P**

856187-83-2P 856188-16-4P 857027-04-4P
857027-05-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

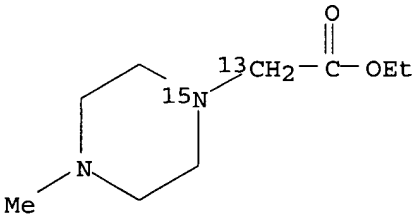
RN 856187-64-9 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



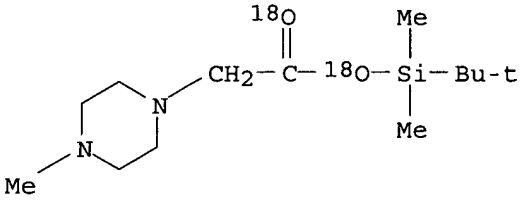
RN 856187-68-3 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



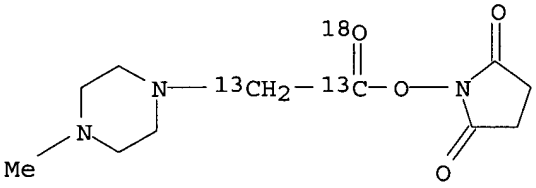
RN 856187-72-9 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 856187-83-2 CAPLUS
CN 1-Piperazineacetic-18O2 acid, 4-methyl-, (1,1-dimethylethyl)dimethylsilyl ester (9CI) (CA INDEX NAME)

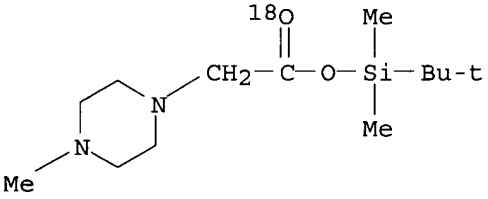


RN 856188-16-4 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

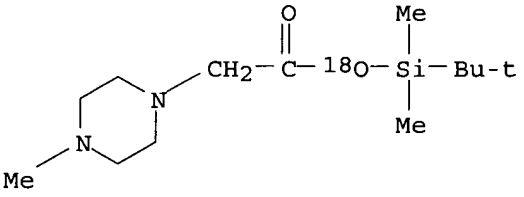


● 2 HCl

RN 857027-04-4 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 16O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)



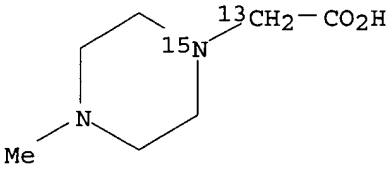
RN 857027-05-5 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 18O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)



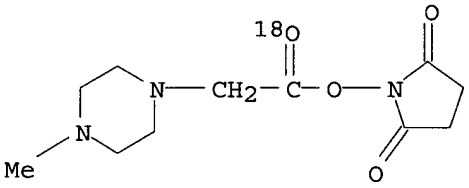
IT **856187-76-3P 856187-87-6P 856187-92-3P**
856290-53-4P 856290-55-6P 857027-11-3P
857027-12-4P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

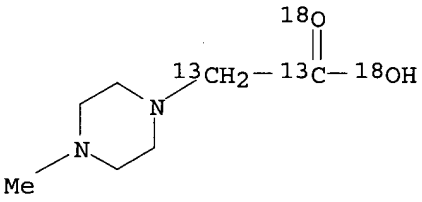
RN 856187-76-3 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-87-6 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)

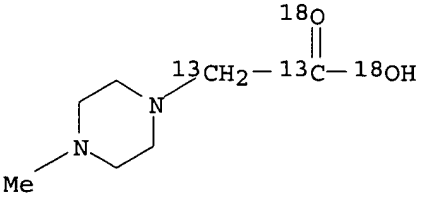


RN 856187-92-3 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

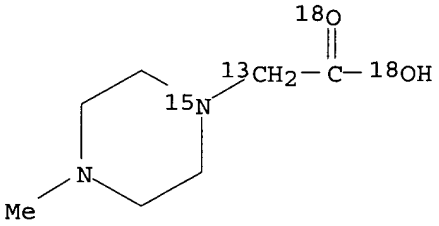


●2 HCl

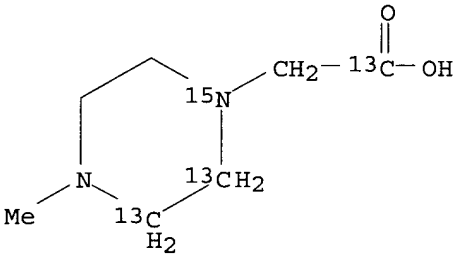
RN 856290-53-4 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



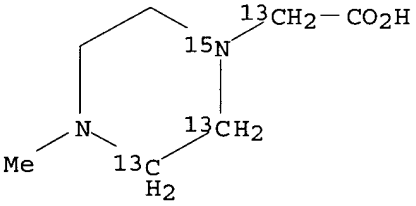
RN 856290-55-6 CAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-11-3 CAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 CAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



L27 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2005:592130 CAPLUS
DOCUMENT NUMBER: 143:115574
TITLE: Preparation of isotopically enriched N-substituted piperazines
INVENTOR(S): **Pappin, Darryl J. C.**; Pillai, Sasi; **Coull, James M.**
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148773	A1	20050707	US 2004-751388	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

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PRIORITY APPLN. INFO.:		
US 2004-751353	A	20040105
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US 2004-751387	A	20040105
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US 2004-822639	A	20040412
US 2004-852730	A	20040524

OTHER SOURCE(S): MARPAT 143:115574

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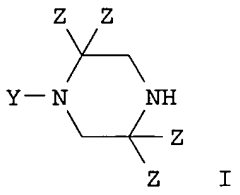


I

AB Isotopically enriched N-substituted piperazines (I) or salts thereof, comprising one or more heavy atom isotopes (Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms; Z = independently H, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H or F atoms, a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms), or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group; wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms; wherein the N-methylpiperazine is isotopically enriched with either of 13C and/or 15N) are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling

reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like (no data). Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

IC ICM C07D241-04

INCL 544358000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 6, 80

IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

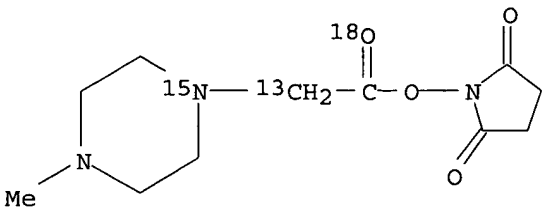
IT 5672-86-6P, Trifluoroacetic acid pentachlorophenyl ester 5672-89-9P, Trifluoroacetic acid succinimidyl ester 54699-92-2P, 4-Methylpiperazine-1-acetic acid 106665-75-2P 145142-98-9P 145143-00-6P 856187-57-0P **856187-64-9P 856187-68-3P 856187-72-9P** 856187-80-9P **856187-83-2P 856187-92-3P 856188-16-4P** 856188-23-3P 856188-27-7P 856188-32-4P 856188-37-9P 856188-43-7P 856188-49-3P 856188-80-2P 856188-88-0P, Trifluoroacetic acid 2-oxopyrrolidin-1-yl ester 856290-54-5P **857027-04-4P 857027-05-5P** 857502-96-6P 857502-97-7P 857502-98-8P 857502-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

IT **856187-76-3P 856187-87-6P** 856188-02-8P, 4-Methylpiperazine-1-acetic acid 1,1,1,3,3,3-hexafluoropropan-2-yl ester 856188-06-2P 856188-38-0P 856188-44-8P 856188-50-6P 856188-62-0P 857027-09-9P 857027-10-2P 857503-00-5P 857503-01-6P 857503-02-7P 857503-03-8P 857503-04-9P 857503-05-0P 857503-06-1P 857503-07-2P 857503-08-3P 857503-09-4P 857503-10-7P 857503-11-8P 857503-12-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856188-20-0 CAPLUS

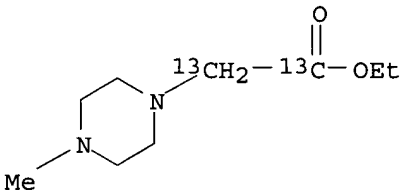
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

IT **856187-64-9P 856187-68-3P 856187-72-9P**
856187-83-2P 856187-92-3P 856188-16-4P
857027-04-4P 857027-05-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856187-64-9 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 856187-68-3 CAPLUS
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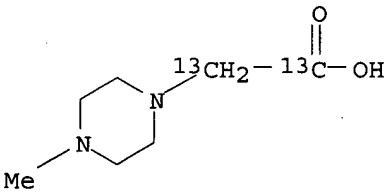
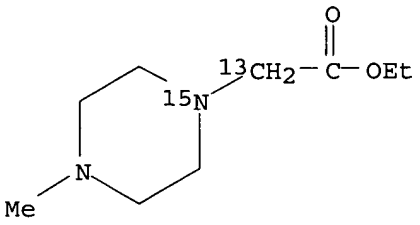
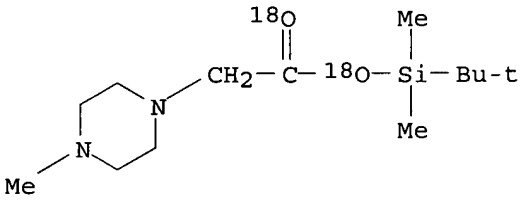


RN 856187-72-9 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 856187-83-2 CAPLUS
CN 1-Piperazineacetic-18O2 acid, 4-methyl-, (1,1-dimethylethyl)dimethylsilyl ester (9CI) (CA INDEX NAME)



RN 856187-92-3 CAPLUS
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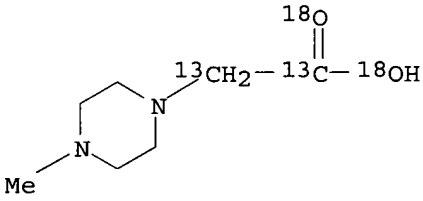
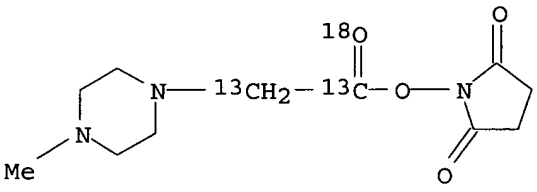


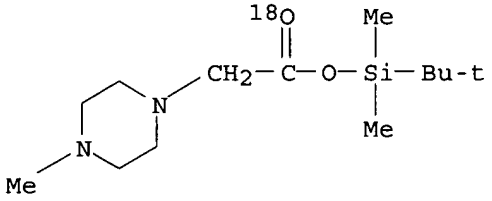
●2 HCl

RN 856188-16-4 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

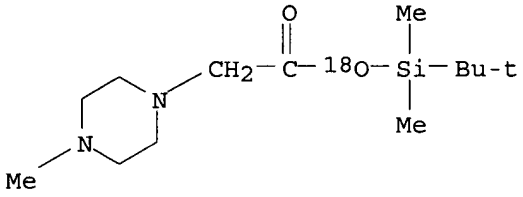


●2 HCl

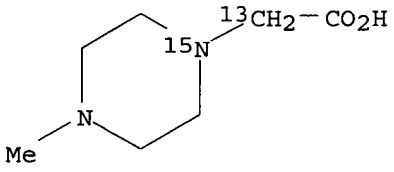
RN 857027-04-4 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 16O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)



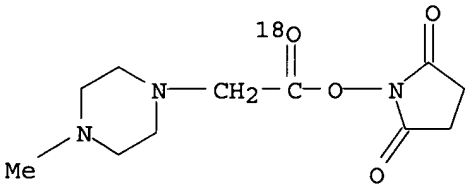
RN 857027-05-5 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 18O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)



IT **856187-76-3P 856187-87-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)
RN 856187-76-3 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-87-6 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



L27 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2005:592129 CAPLUS
DOCUMENT NUMBER: 143:97398
TITLE: Preparation of active esters of N-substituted piperazine acetic acids, including isotopically enriched versions
INVENTOR(S): Dey, Subhakar; **Pappin, Darryl J. C.**; **Purkayastha, Subhasish**; Pillai, Sasi; **Coull, James M.**
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 33 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

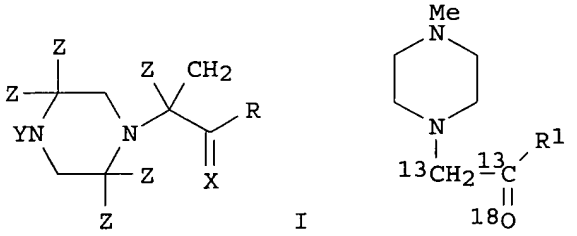
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148771	A1	20050707	US 2004-751354	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A	20040412
US 2004-852730	A	20040524

OTHER SOURCE(S): MARPAT 143:97398
GI



AB In some embodiments, this invention pertains to active esters of N-substituted piperazine acetic acid I (R = leaving group; X = O, S; Y = C1-C6 alkyl, C1-C6 alkyl ether; Z = H, 2H, F, Cl, Br, iodide, amino acid

side chain, C1-C6 alkyl, C1-C6 alkyl ether), including isotopically enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof. For example, the isotopically labeled N-methylpiperazine II (R1 = 18OH) reacted with the trifluoroacetic acid ester of N-hydroxysuccinimide to give the succinate II (R1 = OR2, R2 = succinimido).

IC ICM C07D043-02
ICS C07D241-04

INCL 544182000; 544372000; 544209000; 544371000; 544399000

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

IT **856187-87-6P** 856187-98-9P 856188-02-8P 856188-06-2P **856188-16-4P** **856188-20-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

IT 658-78-6 920-66-1 1737-40-2 4530-20-5, N-Boc-glycine 5672-86-6 5672-89-9 13200-60-7, Sarcosine, ethyl ester 14533-84-7 34352-59-5 54699-92-2 61898-49-5 85539-84-0 856187-95-6 **856188-13-1** 856188-80-2 856188-88-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

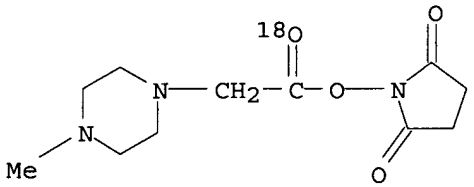
IT 109-01-3P, N-Methylpiperazine 5625-52-5P 145590-97-2P 856187-53-6P 856187-57-0P **856187-64-9P** **856187-68-3P** **856187-72-9P** 856187-80-9P **856187-83-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

IT **856187-76-3P** **856187-92-3P** 856188-23-3P 856188-27-7P 856188-32-4P 856188-38-0P 856188-44-8P 856188-50-6P 856188-62-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

IT **856187-87-6P** **856188-16-4P** **856188-20-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

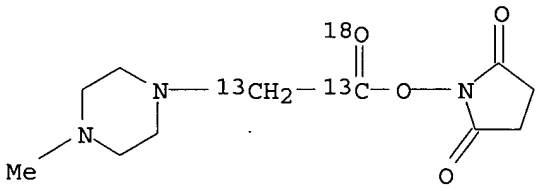
RN 856187-87-6 CAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



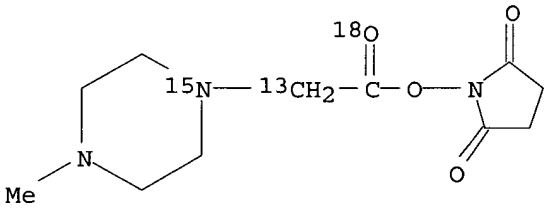
RN 856188-16-4 CAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



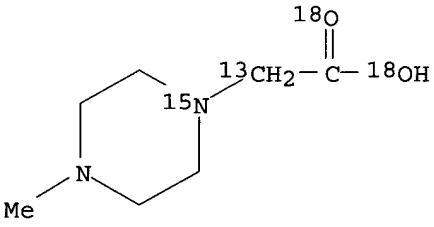
● 2 HCl

RN 856188-20-0 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

IT **856188-13-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)
RN 856188-13-1 CAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

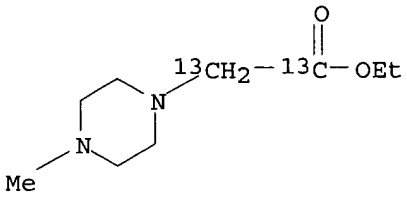


● 2 HCl

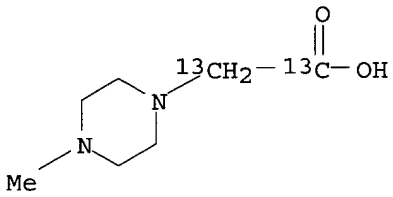
IT **856187-64-9P 856187-68-3P 856187-72-9P**
856187-83-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

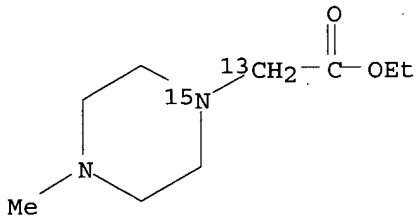
RN 856187-64-9 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



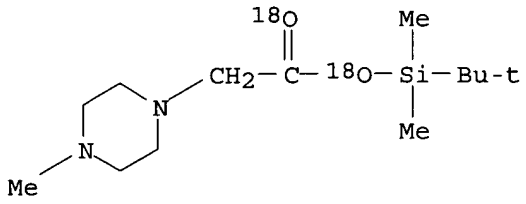
RN 856187-68-3 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



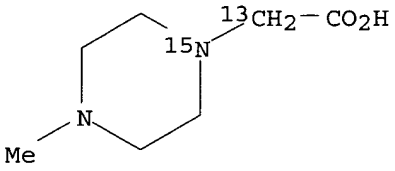
RN 856187-72-9 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



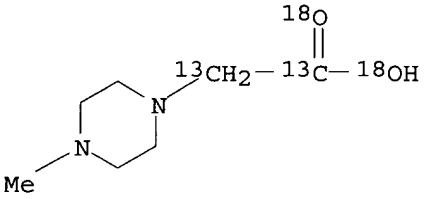
RN 856187-83-2 CAPLUS
CN 1-Piperazineacetic-18O2 acid, 4-methyl-, (1,1-dimethylethyl)dimethylsilyl ester (9CI) (CA INDEX NAME)



IT **856187-76-3P 856187-92-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)
RN 856187-76-3 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-92-3 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L27 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2005:588349 CAPLUS
DOCUMENT NUMBER: 143:112150
TITLE: Isobarically labeled analytes and fragment ions derived therefrom
INVENTOR(S): **Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.**
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S. Ser. No. 822,639.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148087	A1	20050707	US 2004-852730	20040524
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A2 20040105
US 2004-822639	A2 20040412
US 2004-751354	A 20040105
US 2004-751387	A 20040105
US 2004-751388	A 20040105
US 2004-852730	A 20040524

OTHER SOURCE(S): MARPAT 143:112150

AB This invention pertains to isobarically labeled analytes and fragment ions thereof.

IC ICM C07K014-47
ICS C12Q001-68; G01N033-00

INCL 436086000; 530409000

CC 9-16 (Biochemical Methods)

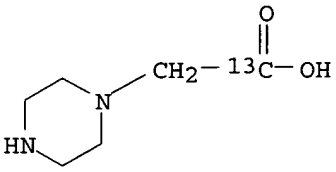
IT 79-08-3DP, Bromoacetic acid, polystyrene trityl chloride piperazine derivs. 110-85-0DP, Piperazine, trityl chloride/bromoacetic polystyrene derivs. 3235-67-4P, 1-Piperidineacetic acid 3235-69-6P, 4-Morpholineacetic acid 5625-52-5P 37478-58-3P, 1-Piperazineacetic acid 53788-49-1P 80841-13-0P 174311-10-5P 215101-76-1P 741683-82-9P, 1-Piperidineacetic-carboxy-13C acid 741683-83-0P, 1-Piperidineacetic-α-13C acid **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid **741683-85-2P**, 1-Piperazineacetic-α-13C acid **856187-64-9P** **856187-72-9P** 856187-80-9P **856187-83-2P** **857027-04-4P** **857027-05-5P** 857027-07-7P 857027-09-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(isobarically labeled analytes and fragment ions derived therefrom)

IT 109-01-3P 34352-59-5P 741683-79-4P 741683-81-8P 856187-57-0P **856187-68-3P** **856187-76-3P** **856187-87-6P** 856187-98-9P 856188-06-2P 856188-62-0P **856290-53-4P** **856290-55-6P** **857027-06-6P** 857027-08-8P 857027-10-2P **857291-36-2P** **857291-38-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(isobarically labeled analytes and fragment ions derived therefrom)

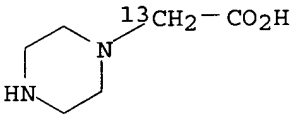
IT **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid **741683-85-2P**, 1-Piperazineacetic-α-13C acid **856187-64-9P** **856187-72-9P** **856187-83-2P** **857027-04-4P** **857027-05-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(isobarically labeled analytes and fragment ions derived therefrom)

RN 741683-84-1 CAPLUS

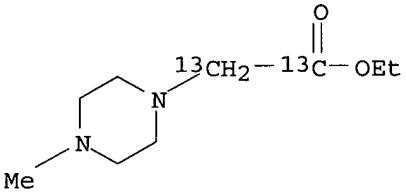
CN 1-Piperazineacetic-carboxy-13C acid (9CI) (CA INDEX NAME)



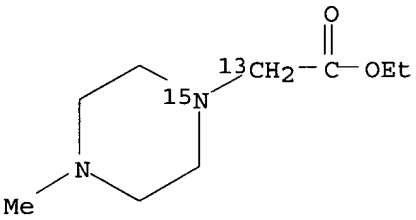
RN 741683-85-2 CAPLUS
CN 1-Piperazineacetic-α-13C acid (9CI) (CA INDEX NAME)



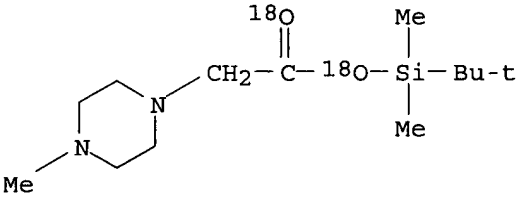
RN 856187-64-9 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI)
(CA INDEX NAME)



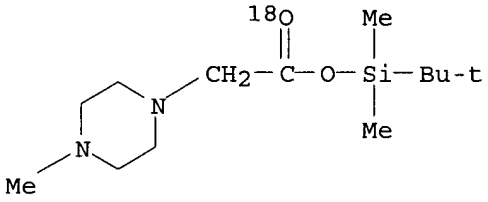
RN 856187-72-9 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI)
(CA INDEX NAME)



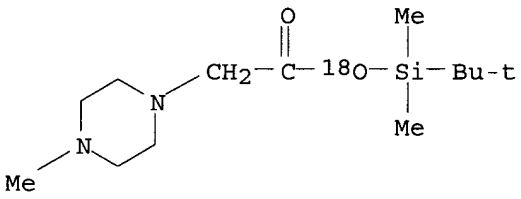
RN 856187-83-2 CAPLUS
CN 1-Piperazineacetic-18O2 acid, 4-methyl-, (1,1-dimethylethyl)dimethylsilyl
ester (9CI) (CA INDEX NAME)



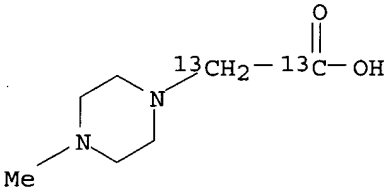
RN 857027-04-4 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 16O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)



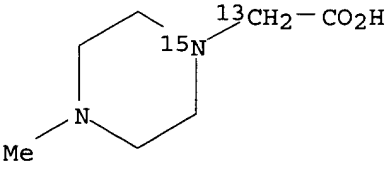
RN 857027-05-5 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 18O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)



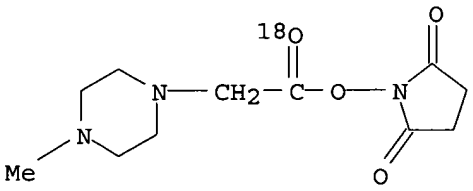
IT **856187-68-3P 856187-76-3P 856187-87-6P**
856290-53-4P 856290-55-6P 857027-06-6P
857291-36-2P 857291-38-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(isobarically labeled analytes and fragment ions derived therefrom)
RN 856187-68-3 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



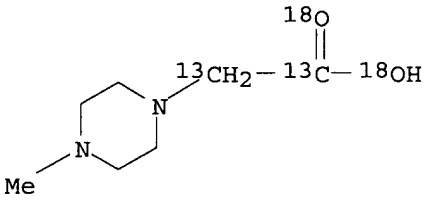
RN 856187-76-3 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



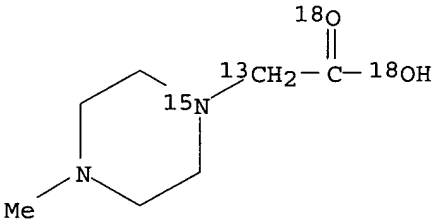
RN 856187-87-6 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



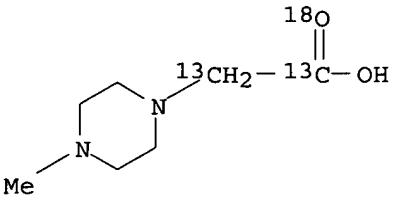
RN 856290-53-4 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856290-55-6 CAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-06-6 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O acid, 4-methyl- (9CI) (CA INDEX NAME)



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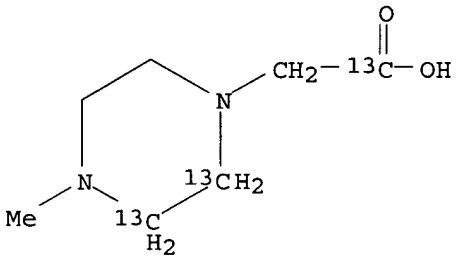
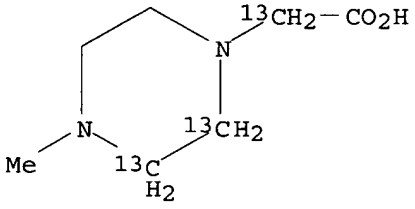
CN 1-Piperazine-2,3-13C2-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX

NAME)



RN 857291-38-4 CAPLUS
CN 1-Piperazine-2,3-13C2-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



L27 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2005:592027 CAPLUS
DOCUMENT NUMBER: 143:93642
TITLE: Mixtures of isobarically labeled analytes and fragments ions derived therefrom
INVENTOR(S): **Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.**
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 751,353.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005147985	A1	20050707	US 2004-822639	20040412
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005148087	A1	20050707	US 2004-852730	20040524
WO 2005068446	A1	20050728	WO 2005-US223	20050105

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,

EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A2	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A2	20040412
US 2004-852730	A	20040524

OTHER SOURCE(S): MARPAT 143:93642

AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.

IC ICM C12Q001-68
ICS C07H021-02; G01N033-00; C07J043-00

INCL 435006000; 436086000; 530409000; 536023100; 540107000; 544359000

CC 9-16 (Biochemical Methods)

IT **856290-53-4P 856290-55-6P 857027-11-3P 857027-12-4P**
RL: FMU (Formation, unclassified); SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

IT 75-89-8 79-08-3, Bromoacetic acid 79-37-8, Ethanedioyl dichloride 139-02-6 771-61-9, Pentafluorophenol 920-66-1 4530-20-5, Boc-Glycine 5672-89-9 6066-82-6 7087-68-5, Diisopropylethylamine 13200-60-7, Sarcosine ethyl ester 18156-74-6 52928-63-9 54699-92-2 56522-24-8 61898-49-5 85539-84-0 99542-20-8 **856187-92-3** 856187-95-6 **856188-13-1** 857027-03-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

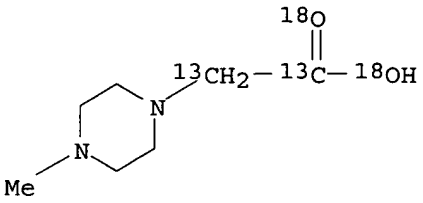
IT 5625-52-5P 53788-49-1P 80841-13-0P 145590-97-2P **856187-64-9P** **856187-68-3P** **856187-72-9P** 856187-80-9P **856187-83-2P** 856188-06-2P **857027-04-4P** **857027-05-5P** 857027-07-7P 857027-09-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

IT 109-01-3P 34352-59-5P 856187-57-0P **856187-76-3P** **856187-87-6P** 856187-98-9P **856188-16-4P** **856188-20-0P** 856188-62-0P **857027-06-6DP**, salts 857027-08-8P 857027-10-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

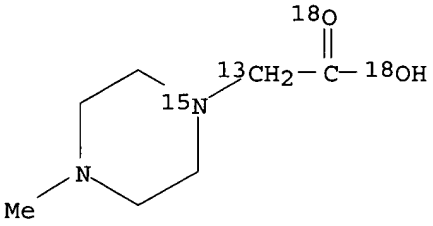
IT **856290-53-4P 856290-55-6P 857027-11-3P 857027-12-4P**
RL: FMU (Formation, unclassified); SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856290-53-4 CAPLUS

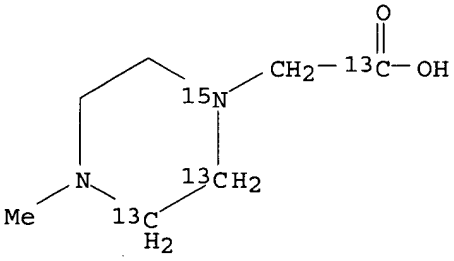
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856290-55-6 CAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-11-3 CAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 CAPLUS
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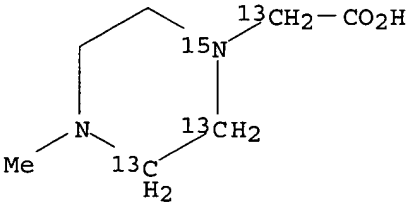
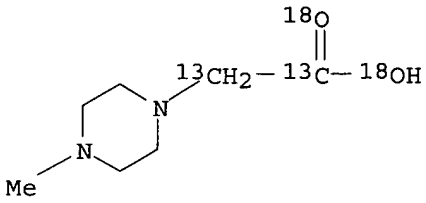


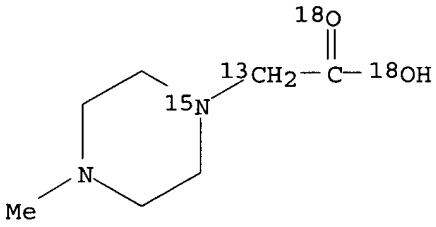
IT **856187-92-3 856188-13-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856187-92-3 CAPLUS

CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



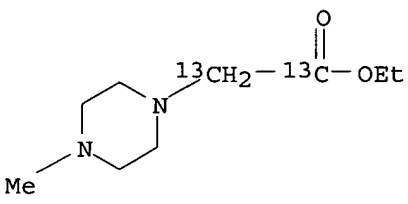
●2 HCl

RN 856188-13-1 CAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

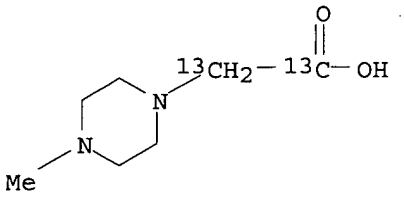


●2 HCl

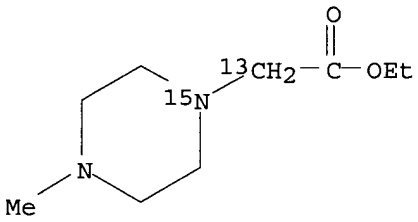
IT **856187-64-9P 856187-68-3P 856187-72-9P**
856187-83-2P 857027-04-4P 857027-05-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856187-64-9 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 856187-68-3 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-72-9 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



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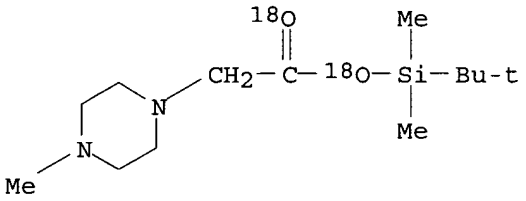
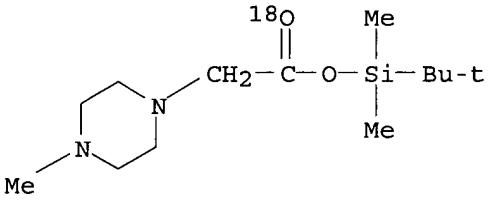
CN 1-Piperazineacetic-18O2 acid, 4-methyl-, (1,1-dimethylethyl)dimethylsilyl ester (9CI) (CA INDEX NAME)



RN 857027-04-4 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 16O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)



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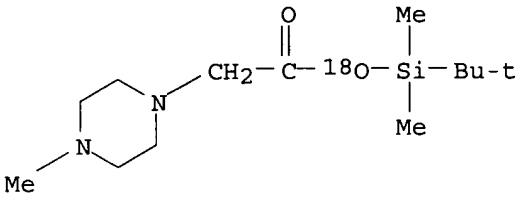
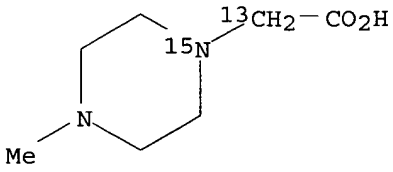
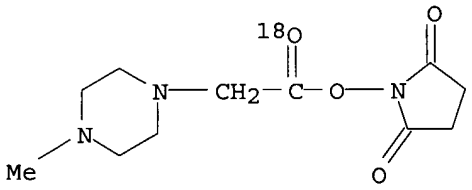


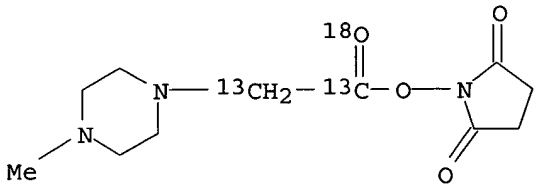
IT **856187-76-3P 856187-87-6P 856188-16-4P**
856188-20-0P 857027-06-6DP, salts
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856187-76-3 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 856187-87-6 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



RN 856188-16-4 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



RN 856188-20-0 CAPLUS
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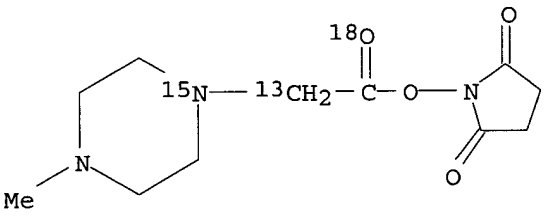
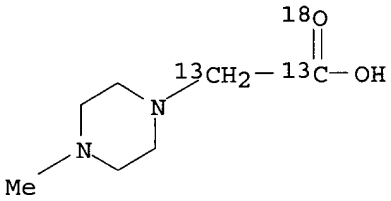


●2 HCl

RN 857027-06-6 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O acid, 4-methyl- (9CI) (CA INDEX NAME)



L27 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 2005:588336 CAPLUS
DOCUMENT NUMBER: 143:93635
TITLE: Mixtures of isobarically labeled analytes and fragments ions derived therefrom
INVENTOR(S): **Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.**
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
US 2005148087	A1	20050707	US 2004-852730	20040524
WO 2005068446	A1	20050728	WO 2005-US223	20050105

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NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
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MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A2 20040105
US 2004-751354	A 20040105
US 2004-751387	A 20040105
US 2004-751388	A 20040105
US 2004-822639	A2 20040412
US 2004-852730	A 20040524

AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.

IC ICM C12Q001-68
ICS C07H021-04; G01N033-00; C07K014-47

INCL 435006000; 436086000; 530409000; 536023100

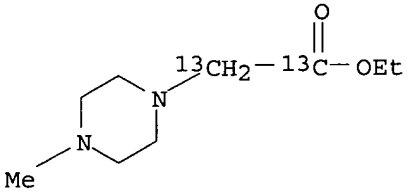
CC 9-16 (Biochemical Methods)

IT 5625-52-5P 53788-49-1P 61898-49-5P, Ethyl bromoacetate 80841-13-0P
145590-97-2P **856187-64-9P** **856187-68-3P**
856187-72-9P 856187-80-9P **856187-83-2P** 856188-06-2P
857027-02-2P **857027-04-4P** **857027-05-5P** 857027-09-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

IT 109-01-3P 34352-59-5P 856187-57-0P **856187-76-3P**
856187-87-6P 856187-98-9P 856188-62-0P **856290-53-4P**
856290-55-6P **857027-06-6DP**, salts 857027-08-8P
857027-10-2P **857027-11-3P** **857027-12-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

IT **856187-64-9P** **856187-68-3P** **856187-72-9P**
856187-83-2P **857027-04-4P** **857027-05-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-64-9 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



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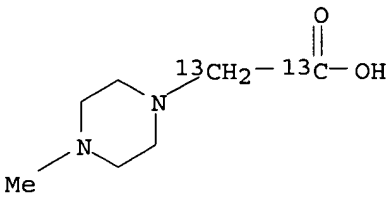
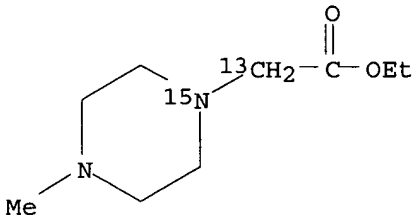
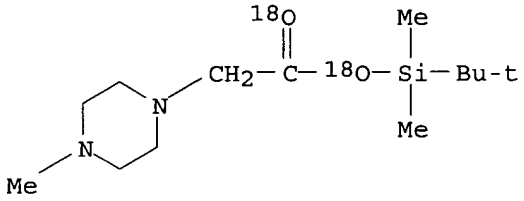
CN 1-Piperazineacetic-carboxy,α-13C2 acid, 4-methyl- (9CI) (CA INDEX NAME)



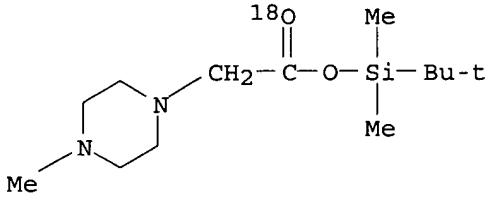
RN 856187-72-9 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



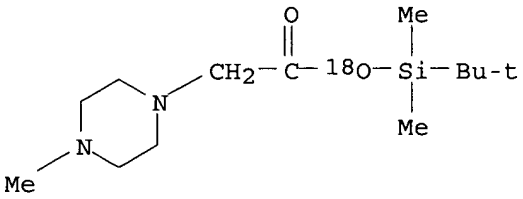
RN 856187-83-2 CAPLUS
CN 1-Piperazineacetic-18O2 acid, 4-methyl-, (1,1-dimethylethyl)dimethylsilyl ester (9CI) (CA INDEX NAME)



RN 857027-04-4 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 16O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)

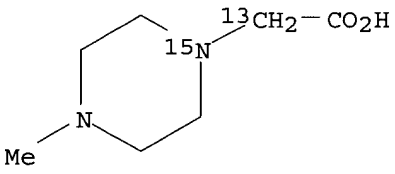


RN 857027-05-5 CAPLUS
CN 1-Piperazineacetic-18O acid, 4-methyl-, 18O-[(1,1-dimethylethyl)dimethylsilyl] ester (9CI) (CA INDEX NAME)

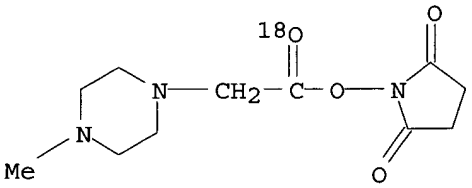


IT **856187-76-3P 856187-87-6P 856290-53-4P**
856290-55-6P 857027-06-6DP, salts **857027-11-3P**
857027-12-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

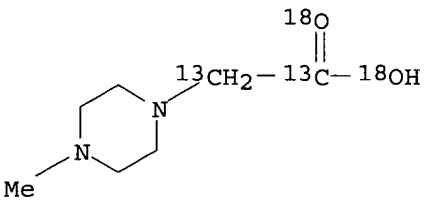
RN 856187-76-3 CAPLUS
CN 1-Piperazine-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



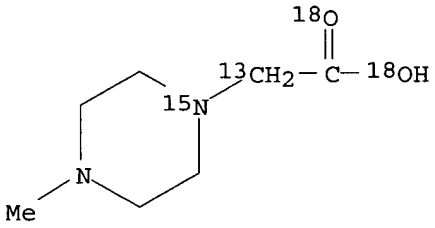
RN 856187-87-6 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



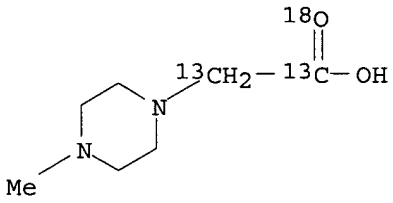
RN 856290-53-4 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



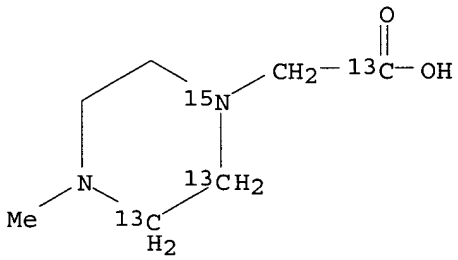
RN 856290-55-6 CAPLUS
CN 1-Piperazineacetic-α-13C-1-15N-18O2 acid, 4-methyl- (9CI) (CA INDEX NAME)



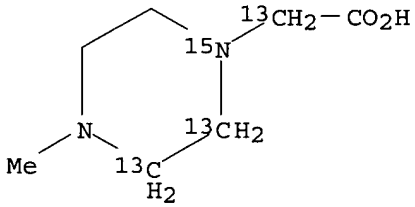
RN 857027-06-6 CAPLUS
CN 1-Piperazineacetic-carboxy,α-13C2-18O acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-11-3 CAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-carboxy-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



RN 857027-12-4 CAPLUS
CN 1-Piperazine-2,3-13C2-1-15N-acetic-α-13C acid, 4-methyl- (9CI) (CA INDEX NAME)



L27 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:523758 CAPLUS

DOCUMENT NUMBER: 143:56140
TITLE: Analysis of mass spectral data in the quiet zones using label fragment ions and applications in analysis of proteins and other biomolecules
INVENTOR(S): **Pappin, Darryl J. C.**
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005054871	A2	20050616	WO 2004-US41343	20041124
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005153456	A1	20050714	US 2004-999638	20041126
PRIORITY APPLN. INFO.:			US 2003-525478P P	20031126
			US 2004-547375P P	20040224

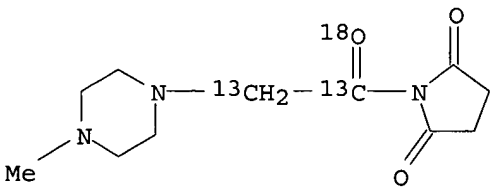
OTHER SOURCE(S): MARPAT 143:56140

AB The invention pertains to methods, systems and/or compns. useful for the anal. of labels and/or labeled analytes in quiet zones. Because the labeling reagents can be isotopically enriched, label fragment ions generated by fragmentation of a label in a mass spectrometer can produce an isotopic cluster of distinct peak configuration. The labeling reagents that fragment to produce the isotopic clusters observed in the mass spectrum can be directed to "quiet zones" across a mass spectrum. The "quiet zones" are areas where little or no mass intensity information exists in the summed result for the analyte type or types. By directing the anal. to the quiet zones, where few or no analyte fragment ions are detected, it is possible to improve the reliability of any qual. and/or quant. anal. of the label based on determination of the label fragment ions. The method can be used for mass spectrometric anal. of proteins, peptides, lipids, nucleic acids, carbohydrates or small mols.

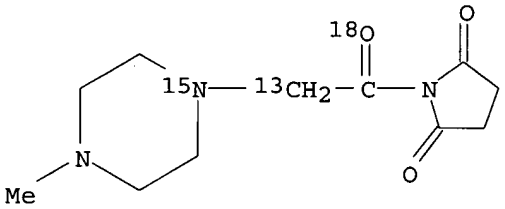
IC ICM G01N033-68
ICS C07D211-40; C07D211-10; C07D211-56; C07F009-00; C07D265-00; C07D279-00; C07D217-00
CC 9-5 (Biochemical Methods)
IT **853995-43-4 853995-44-5 853995-45-6 853995-46-7**
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(anal. of mass spectral data in quiet zones using label fragment ions and applications in anal. of proteins and other biomols.)
IT **853995-43-4 853995-44-5 853995-45-6 853995-46-7**
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)

(anal. of mass spectral data in quiet zones using label fragment ions and applications in anal. of proteins and other biomols.)

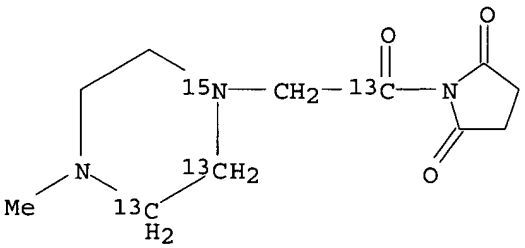
RN 853995-43-4 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl)acetyl-13C2-18O]- (9CI) (CA INDEX NAME)



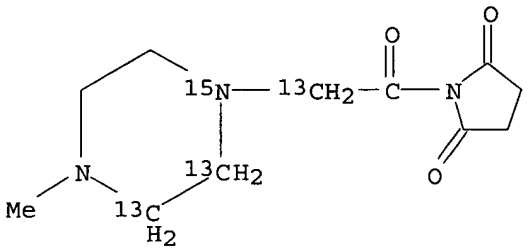
RN 853995-44-5 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]- (9CI) (CA INDEX NAME)



RN 853995-45-6 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-1-13C]- (9CI) (CA INDEX NAME)



RN 853995-46-7 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-2-13C]- (9CI) (CA INDEX NAME)



L27 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:371290 CAPLUS
DOCUMENT NUMBER: 142:409686
TITLE: Method of reducing leachate released in protein A-based affinity purification of antibodies
INVENTOR(S): Leete, Thomas D.; Creasey, Theresa S.; Smith, Robert; **Coull, James M.; Pappin, Darryl J.**; Mccoy, Mark A.
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037869	A2	20050428	WO 2004-US34249	20041015
WO 2005037869	A3	20050616		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005165222	A1	20050728	US 2004-966188	20041015

PRIORITY APPLN. INFO.: US 2003-511521P P 20031015

AB The disclosed invention provides methods and compns. used for antibody purification by protein A-based affinity techniques. In particular, methods are provided for reducing the levels of protein A leachate in such affinity-purified antibody prepns. In addition, the present invention relates to protein A affinity chromatog. binding buffer compns. and to antibody compns. In the example, protein A chromatog. was performed using a customized PerSeptive BioCad 700E HPLE system equipped with a stainless steel column (4.6 mm X 10 cm) containing a bed of POROS A50 resin (protein A affinity support from Applied Biosystems). The antibody sample loaded on the equilibrated POROS A50 column is human serum IgG. The inventors also measured the protein A leachate concns. using a protein A ELISA kit, and quantified the protease activity using a suitable enzyme assay.

IC ICM C07K016-06
ICS C07K001-22

CC 15-1 (Immunochemistry)
Section cross-reference(s): 9

L27 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:681717 CAPLUS
DOCUMENT NUMBER: 141:202794
TITLE: Methods, mixtures, kits and compositions pertaining to analyte determination
INVENTOR(S): **Pappin, Darryl J. C.**; Bartlet-Jones, Michael
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

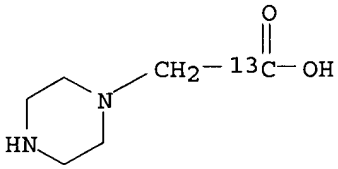
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004070352	A2	20040819	WO 2004-US2077	20040127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2488584	AA	20040819	CA 2004-2488584	20040127
US 2004219685	A1	20041104	US 2004-765264	20040127
US 2004220412	A1	20041104	US 2004-765267	20040127
US 2004219686	A1	20041104	US 2004-765458	20040127
EP 1588145	A2	20051026	EP 2004-705571	20040127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: US 2003-443612P P 20030130
WO 2004-US2077 W 20040127

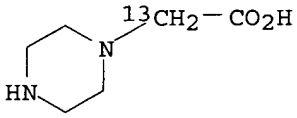
AB This invention pertains to methods, mixts., kits and/or compns. for the determination of analytes by mass anal. using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixts. suitable for multiplex anal. of the labeled analytes.

IC ICM G01N
CC 9-16 (Biochemical Methods)
IT 3235-67-4P, 1-Piperidineacetic acid 3235-69-6P, 4-Morpholineacetic acid 37478-58-3P, 1-Piperazineacetic acid 215101-76-1P 741683-82-9P, 1-Piperidineacetic-carboxy-13C acid 741683-83-0P, 1-Piperidineacetic-α-13C acid **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid **741683-85-2P**, 1-Piperazineacetic-α-13C acid 741683-87-4P, 4-Morpholineacetic-carboxy-13C acid 741683-88-5P, 4-Morpholineacetic-α-13C acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(methods, mixts., kits and compns. pertaining to analyte determination)
IT **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid
741683-85-2P, 1-Piperazineacetic-α-13C acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(methods, mixts., kits and compns. pertaining to analyte determination)
RN 741683-84-1 CAPLUS
CN 1-Piperazineacetic-carboxy-13C acid (9CI) (CA INDEX NAME)



RN 741683-85-2 CAPLUS
CN 1-Piperazineacetic-α-13C acid (9CI) (CA INDEX NAME)



L27 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:19284 CAPLUS
DOCUMENT NUMBER: 142:257250
TITLE: Multiplexed protein quantitation in Saccharomyces cerevisiae using amine-reactive isobaric tagging reagents
AUTHOR(S): Ross, Philip L.; Huang, Yulin N.; Marchese, Jason N.; Williamson, Brian; Parker, Kenneth; Hattan, Stephen; Khainovski, Nikita; Pillai, Sasi; Dey, Subhakar; Daniels, Scott; **Purkayastha, Subhasish**; Juhasz, Peter; Martin, Stephen; Bartlet-Jones, Michael; He, Feng; Jacobson, Allan; **Pappin, Darryl J.**
CORPORATE SOURCE: Applied Biosystems, Framingham, MA, 01701, USA
SOURCE: Molecular and Cellular Proteomics (2004), 3(12), 1154-1169
CODEN: MCPOBS; ISSN: 1535-9476
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We describe here a multiplexed protein quantitation strategy that provides relative and absolute measurements of proteins in complex mixts. At the core of this methodol. is a multiplexed set of isobaric reagents that yield amine-derivatized peptides. The derivatized peptides are indistinguishable in MS, but exhibit intense low-mass MS/MS signature ions that support quantitation. In this study, we have examined the global protein expression of a wild-type yeast strain and the isogenic upf1Δ and xrn1Δ mutant strains that are defective in the nonsense-mediated mRNA decay and the general 5' to 3' decay pathways, resp. We also demonstrate the use of 4-fold multiplexing to enable relative protein measurements simultaneously with determination of absolute levels of a target protein using synthetic isobaric peptide stds. We find that inactivation of Upf1p and Xrn1p causes common as well as unique effects on

protein expression.
CC 9-16 (Biochemical Methods)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:425568 CAPLUS
DOCUMENT NUMBER: 115:25568
TITLE: Immobilization of proteins and peptides on insoluble supports for sequencing and other applications
INVENTOR(S): **Pappin, Darryl J. C.**; **Coull, James M.**; Koester, Hubert
PATENT ASSIGNEE(S): Millipore Corp., USA
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 410323	A2	19910130	EP 1990-113972	19900720
EP 410323	A3	19920408		
R: DE, FR, GB, IT, NL, SE				
US 5071909	A	19911210	US 1989-385711	19890726
JP 03141300	A2	19910617	JP 1990-194113	19900724

PRIORITY APPLN. INFO.: US 1989-385711 A 19890726
AB A peptide or protein is immobilized onto a flat, microporous membrane by (1) adsorbing the peptide or protein and a crosslinkable polymer onto the membrane surface, and (2) crosslinking the polymer to produce a polymer network entrapping the protein or peptide therein. The immobilized peptide or protein is suitable for sequence anal. or other chemical or enzymic processes. Thus, a polyvinylidene difluoride membrane disk containing electroblotted β-lactoglobulin A and stained with sulforhodamine B was treated with diisopropyl-carbodiimide and methylenedianiline (polymer crosslinking agent), dried, then treated with polyacrylic acid (5000 mol. weight). The prepared disk was subjected to 20 cycles of Edman degradation The initial sequencing yield was 35 pmol and the repetitive yield 90%.
IC ICM G01N033-68
ICA G01N033-549; G01N033-545
CC 9-15 (Biochemical Methods)
Section cross-reference(s): 34

L27 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:240863 CAPLUS
DOCUMENT NUMBER: 114:240863
TITLE: Identification of phosphorylated sites in the mouse glucocorticoid receptor
AUTHOR(S): Bodwell, Jack E.; Orti, Eduardo; **Coull, James M.**; **Pappin, Darryl J. C.**; Smith, Lynda I.; Swift, Fiona
CORPORATE SOURCE: Dep. Physiol., Dartmouth Med. Sch., Hanover, NH, 03756, USA
SOURCE: Journal of Biological Chemistry (1991), 266(12), 7549-55
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Glucocorticoid receptors in vivo are phosphorylated in the absence of hormone and become hyperphosphorylated in the presence of glucocorticoid agonist but not antagonists (Orti, E., et al., 1989). As a preliminary step to elucidating the functional significance of receptor phosphorylation, phosphorylated sites were identified on the mouse receptor. Tryptic phosphopeptides from 32P-labeled receptors were purified from glucocorticoid-treated mouse thymoma cells (WEHI-7) and from stably transfected Chinese hamster ovary cells (WCL2) that express large nos. of mouse receptors. Phosphopeptide maps of receptors from these 2 cell types were almost indistinguishable. Solid phase sequencing revealed phosphorylation at serines 122, 150, 212, 220, 234, and 315 and threonine 159. Serines 122, 150, 212, 220, and 234 and the sequences surrounding them are conserved in the homologous regions of the rat and human receptors, but threonine 159 and serine 315 have no homologues in the human receptor. The 7 phosphorylated sites are in the amino-terminal domain of the receptor. All but serine 315 are within transactivation domains identified in the human and/or rat receptors. Serines 212, 220, and 234 are in a highly acidic region that in the mouse receptor is necessary for full transcription initiation activity and reduces nonspecific DNA binding. Serines 212, 220, and 234 and threonine 159 are in consensus sequences for proline-directed kinase and/or p34cdc2 kinase. Serine 122 is in a consensus sequence for casein kinase II whereas serines 150 and 315 do not appear to be in any known kinase consensus sequence. The location of many of these sites suggests a role of phosphorylation in transactivation.

CC 2-4 (Mammalian Hormones)

L27 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:243669 CAPLUS

DOCUMENT NUMBER: 114:243669

TITLE: Functionalized membrane supports for covalent protein microsequence analysis

AUTHOR(S): **Coull, James M.; Pappin, Darryl J. C.**; Mark, Jonathan; Aebersold, Ruedi; Koster, Hubert

CORPORATE SOURCE: MilliGen/Bios., Div. Millipore, Burlington, MA, 01803, USA

SOURCE: Analytical Biochemistry (1991), 194(1), 110-20
CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Methods were developed for high-yield covalent attachment of peptides and proteins to isothiocyanate and arylamine-derivatized poly(vinylidene difluoride) membranes for solid-phase sequence anal. Solns. of protein or peptide were dried onto 8-mm membrane disks such that the functional groups on the surface and the polypeptide were brought into close proximity. In the case of the isothiocyanate membrane, reaction between polypeptide amino groups and the surface isothiocyanate moieties was promoted by application of aqueous N-methylmorpholine. Attachment of proteins and peptides to the arylamine surface was achieved by application of water-soluble carbodiimide in a pH 5.0 buffer. Edman degradation of covalently bound polypeptides was accomplished with initial and repetitive sequence yields ranging 33-75% and 88.5-98.5%, resp. The yields were independent of the sample load (20 pmol to >1 nmol) for either surface. Significant loss of material was not observed when attachment residues were encountered during sequence runs. Application of bovine β-lactoglobulin A chain, staphylococcus protein A, or the peptide melittin to the isothiocyanate membrane allowed for extended N-terminal sequence identification (35

residues from 20 pmol of β-lactoglobulin). Several synthetic and naturally occurring peptides were sequenced to the C-terminal residue following attachment to the arylamine surface. In 1 example, 10 μg of bovine α-casein was digested with staphylococcal protease V8 and the peptides were separated by reversed-phase chromatog. Peptide fractions were then directly applied to arylamine membrane disks for covalent sequence anal. From as little as 2 pmol of initial signal it was possible to determine substantial sequence information (>10 residues).
CC 9-3 (Biochemical Methods)

L27 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:627543 CAPLUS
DOCUMENT NUMBER: 113:227543
TITLE: Membranes for solid phase protein sequencing
INVENTOR(S): **Coull, James M.; Pappin, Darryl J. C.**; Koster, Hubert; Pluskal, Malcolm G.; Steuck, Michael J.; Bonner, Alex G.
PATENT ASSIGNEE(S): Millipore Corp., USA
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 353460	A2	19900207	EP 1989-111792	19890628
EP 353460	A3	19910904		
R: DE, FR, GB, IT, NL, SE				
US 5011861	A	19910430	US 1988-212430	19880628
JP 02045537	A2	19900215	JP 1989-164115	19890628
JP 2796599	B2	19980910		

PRIORITY APPLN. INFO.: US 1988-212430 A 19880628
AB A membrane suitable for immobilizing peptides and proteins is disclosed. The membrane is a flexible, polymeric, porous membrane (preferably a polymeric fluorocarbon) which contains functional groups capable of covalently linking peptides and proteins. The functional groups can be provided by reacting the membrane itself or a coating thereon with nucleophiles which provide amino, mercapto, hydroxyl, or carboxyl functionality to the membrane surface. Addnl., surfaces containing amino groups can be further reacted with diisothiocyanates to provide an isothiocyanate functionality having enhanced covalent binding characteristics. A particularly preferred membrane for protein sequencing is a poly(vinylidene difluoride) membrane coated with crosslinked hydroxypropyl acrylate having isothiocyanate functional groups. The above membrane was prepared by activating a 2-hydroxypropyl acrylate-coated poly(vinylidene difluoride) membrane (DVPP membrane, Millipore) with 1,1'-carbonyl diimidazole, reacting the activated membrane with 1,3-diaminopropane, and then reacting the amino functionalized membrane with 1,3-phenylene diisothiocyanate. Horse heart myoglobin was immobilized on the thus-prepared membrane, and was sequenced in an automated solid-phase sequencer using 30 cycles of Edman degradation (Laursen, R. A.; 1971).
IC ICM C07K017-02
ICS G01N033-68
ICA B01D067-00; B01D069-00
CC 9-2 (Biochemical Methods)
Section cross-reference(s): 35

L27 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:467672 CAPLUS
DOCUMENT NUMBER: 115:67672
TITLE: New approaches to covalent sequence analysis
AUTHOR(S): **Pappin, Darryl J. C.**; **Coull, James M.**; Koester, Hubert
CORPORATE SOURCE: MilliGen/Biosearch Div., Millipore, Burlington, MA, 01803, USA
SOURCE: Curr. Res. Protein Chem.: Tech., Struct., Funct., [Pap. Annu. Symp. Protein Soc.], 3rd (1990), Meeting Date 1989, 191-202. Editor(s): Villafranca, Joseph J. Academic: San Diego, Calif.
CODEN: 56XQAW
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A symposium report on covalent (solid-phase) sequence anal. of proteins. Thus, peptides or proteins are blotted onto an underivatized polyvinylidene membranes, stained by conventional techniques, and then efficiently covalently immobilized to the membrane surface by entrapment in a thin polymer coating.
CC 9-1 (Biochemical Methods)

L27 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:420480 CAPLUS
DOCUMENT NUMBER: 113:20480
TITLE: Solid-phase sequence analysis of proteins electroblotted or spotted onto polyvinylidene difluoride membranes
AUTHOR(S): **Pappin, Darryl J. C.**; **Coull, James M.**; Koster, Hubert
CORPORATE SOURCE: MilliGen/Biosearch, Burlington, MA, 01803, USA
SOURCE: Analytical Biochemistry (1990), 187(1), 10-19
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Electroblotted proteins noncovalently bound to polyvinylidene difluoride (PVDF) membranes are typically sequenced using adsorptive sequencer protocols (gas phase or pulsed-liquid) that do not require a covalent linkage between protein and surface. Simple chemical protocols were developed where proteins are first electroblotted onto unmodified PVDF membranes, visualized with common protein stains, and then immobilized for solid-phase sequence anal. Adsorbed, stained proteins are first treated with phenylisothiocyanate (PITC) to modify α and ε amines. The protein is then overlayed with a solution of 1,4-phenylene diisothiocyanate (DITC), followed by a few microliters of a basic solution containing a poly(alkylamine). As the polymer dries onto the surface both polymer and remaining protein amino groups are crosslinked by DITC. The protein is thus immobilized to the membrane surface by entrapment in a thin polymer coating. The coating is transparent to the degradation chemical, and extensive enough to remain immobilized even in the absence of any covalent link between polymer and surface. Partial modification with PITC allows for identification of N-terminal and internal lysine residues during sequencing. The process was tested with a variety of poly(alkylamines), linear and branched, with mol. wts. ranging from 600 to >100,000. Proteins bound in this manner were successfully sequenced using covalent (solid-phase) sequencer protocols with cyclic times as short as 26 min.
CC 9-15 (Biochemical Methods)

L27 ANSWER 17 OF 22 USPATFULL on STN
ACCESSION NUMBER: 2005:190304 USPATFULL
TITLE: Method of reducing leachate from protein a affinity media
INVENTOR(S): Leete, Thomas D., Westford, MA, UNITED STATES
Creasey, Theresa S., Bedford, MA, UNITED STATES
Smith, Robert M., Stow, MA, UNITED STATES
Coull, James M., Westford, MA, UNITED STATES
Pappin, Darryl J., Boxborough, MA, UNITED STATES
Edwards, Brooks, Cambridge, MA, UNITED STATES
McCoy, Mark A., Framingham, MA, UNITED STATES
PATENT ASSIGNEE(S): Applera Corporation, Foster City, CA, UNITED STATES, 94404 (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2005165222	A1	20050728
APPLICATION INFO.:	US 2004-966188	A1	20041015 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2003-511521P	20031015 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MILA KASAN, PATENT DEPT., APPLIED BIOSYSTEMS, 850 LINCOLN CENTRE DRIVE, FOSTER CITY, CA, 94404, US
NUMBER OF CLAIMS: 27
EXEMPLARY CLAIM: 1
LINE COUNT: 608
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Disclosed are methods and compositions that may be used for purifying antibodies.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L27 ANSWER 18 OF 22 USPATFULL on STN
ACCESSION NUMBER: 2005:177376 USPATFULL
TITLE: Analysis of mass spectral data in the quiet zones
INVENTOR(S): **Pappin, Darryl J.C.**, Boxborough, MA, UNITED STATES
PATENT ASSIGNEE(S): Applera Corporation, Framingham, MA, UNITED STATES (U.S. corporation)

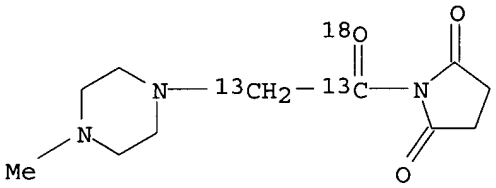
	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2005153456	A1	20050714
APPLICATION INFO.:	US 2004-999638	A1	20041126 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2003-525478P	20031126 (60)
	US 2004-547375P	20040224 (60)

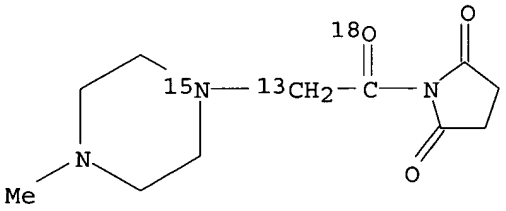
DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: APPLIED BIOSYSTEMS, 500 OLD CONNECTICUT PATH, FRAMINGHAM, MA, 01701, US
NUMBER OF CLAIMS: 35
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 6 Drawing Page(s)
LINE COUNT: 699
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Embodiments of this invention relate to the analysis of mass spectral data in the quiet zones.

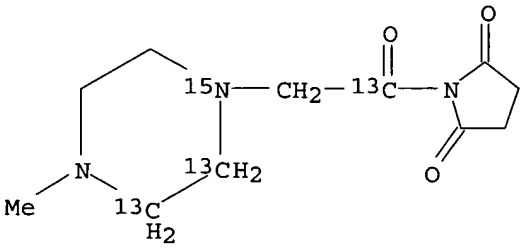
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **853995-43-4 853995-44-5 853995-45-6**
853995-46-7
(anal. of mass spectral data in quiet zones using label fragment ions and applications in anal. of proteins and other biomols.)
RN 853995-43-4 USPATFULL
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl)acetyl-13C2-18O]- (9CI) (CA INDEX NAME)



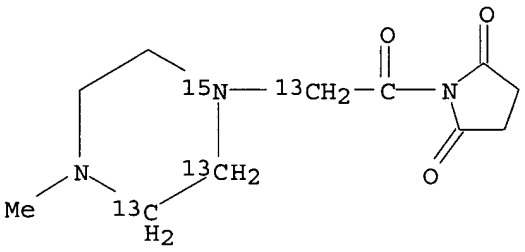
RN 853995-44-5 USPATFULL
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]- (9CI) (CA INDEX NAME)



RN 853995-45-6 USPATFULL
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-1-13C]- (9CI) (CA INDEX NAME)



RN 853995-46-7 USPATFULL
CN 2,5-Pyrrolidinedione, 1-[(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-2-13C]- (9CI) (CA INDEX NAME)



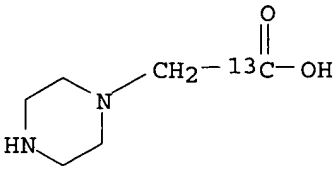
L27 ANSWER 19 OF 22 USPATFULL on STN
ACCESSION NUMBER: 2004:281111 USPATFULL
TITLE: Compositions and kits pertaining to analyte determination
INVENTOR(S): **Pappin, Darryl J.C.**, Boxborough, MA, UNITED STATES
Bartlet-Jones, Michael, Worcester Park, UNITED KINGDOM
PATENT ASSIGNEE(S): Apple Corporation (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004220412	A1	20041104
APPLICATION INFO.:	US 2004-765267	A1	20040127 (10)

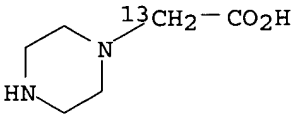
	NUMBER	DATE
PRIORITY INFORMATION:	US 2003-443612P	20030130 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: BRIAN D. GILDEA, APPLIED BIOSYSTEMS, 15 DEANGELO DRIVE, BEDFORD, MA, 01730
NUMBER OF CLAIMS: 70
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 13 Drawing Page(s)
LINE COUNT: 2502
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention pertains to methods, mixtures, kits and/or compositions for the determination of analytes by mass analysis using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixtures suitable for multiplex analysis of the labeled analytes.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid
741683-85-2P, 1-Piperazineacetic-α-13C acid
(methods, mixts., kits and compns. pertaining to analyte determination)
RN 741683-84-1 USPATFULL
CN 1-Piperazineacetic-carboxy-13C acid (9CI) (CA INDEX NAME)



RN 741683-85-2 USPATFULL
CN 1-Piperazineacetic-α-13C acid (9CI) (CA INDEX NAME)



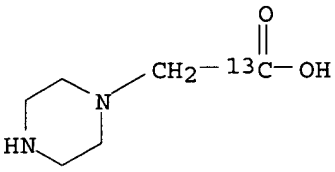
L27 ANSWER 20 OF 22 USPATFULL on STN
ACCESSION NUMBER: 2004:280386 USPATFULL
TITLE: Methods and mixtures pertaining to analyte determination
INVENTOR(S): **Pappin, Darryl J.C.**, Boxborough, MA, UNITED STATES
Bartlet-Jones, Michael, Worcester Park, UNITED KINGDOM

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004219686	A1	20041104
APPLICATION INFO.:	US 2004-765458	A1	20040127 (10)

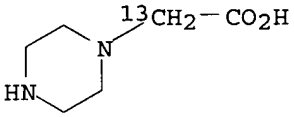
	NUMBER	DATE
PRIORITY INFORMATION:	US 2003-443612P	20030130 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: BRIAN D. GILDEA, APPLIED BIOSYSTEMS, 15 DEANGELO DRIVE, BEDFORD, MA, 01730
NUMBER OF CLAIMS: 110
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 13 Drawing Page(s)
LINE COUNT: 2896
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention pertains to methods, mixtures, kits and/or compositions for the determination of analytes by mass analysis using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixtures suitable for multiplex analysis of the labeled analytes.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid
741683-85-2P, 1-Piperazineacetic-α-13C acid
(methods, mixts., kits and compns. pertaining to analyte determination)
RN 741683-84-1 USPATFULL
CN 1-Piperazineacetic-carboxy-13C acid (9CI) (CA INDEX NAME)



RN 741683-85-2 USPATFULL
CN 1-Piperazineacetic-α-13C acid (9CI) (CA INDEX NAME)



L27 ANSWER 21 OF 22 USPATFULL on STN

ACCESSION NUMBER:	2004:280385 USPATFULL
TITLE:	Methods and mixtures pertaining to analyte determination using electrophilic labeling reagents
INVENTOR(S):	**Pappin, Darryl J.C.**, Boxborough, MA, UNITED STATES Bartlet-Jones, Michael, Worcester Park, UNITED KINGDOM
PATENT ASSIGNEE(S):	Applera Corporation (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004219685	A1	20041104
APPLICATION INFO.:	US 2004-765264	A1	20040127 (10)

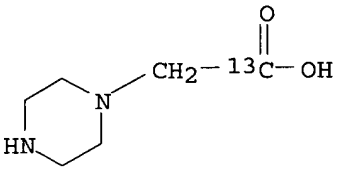
	NUMBER	DATE
PRIORITY INFORMATION:	US 2003-443612P	20030130 (60)

DOCUMENT TYPE:	Utility
FILE SEGMENT:	APPLICATION
LEGAL REPRESENTATIVE:	BRIAN D. GILDEA, APPLIED BIOSYSTEMS, 15 DEANGELO DRIVE, BEDFORD, MA, 01730
NUMBER OF CLAIMS:	114
EXEMPLARY CLAIM:	1
NUMBER OF DRAWINGS:	13 Drawing Page(s)
LINE COUNT:	2776

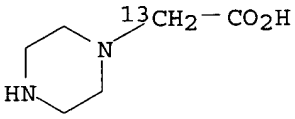
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention pertains to methods, mixtures, kits and/or compositions for the determination of analytes by mass analysis using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixtures suitable for multiplex analysis of the labeled analytes.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **741683-84-1P**, 1-Piperazineacetic-carboxy-13C acid
741683-85-2P, 1-Piperazineacetic-α-13C acid
(methods, mixts., kits and compns. pertaining to analyte determination)
RN 741683-84-1 USPATFULL
CN 1-Piperazineacetic-carboxy-13C acid (9CI) (CA INDEX NAME)



RN 741683-85-2 USPATFULL
CN 1-Piperazineacetic-α-13C acid (9CI) (CA INDEX NAME)



L27 ANSWER 22 OF 22 USPATFULL on STN
ACCESSION NUMBER: 91:100423 USPATFULL
TITLE: Immobilization of proteins and peptides on insoluble supports
INVENTOR(S): **Pappin, Darryl J. C.**, West Concord, MA, United States
Coull, James M., Acton, MA, United States
Koester, Hubert, Concord, MA, United States
PATENT ASSIGNEE(S): Millipore Corporation, Bedford, MA, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 5071909		19911210	
APPLICATION INFO.:	US 1989-385711		19890726	(7)

DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Page, Thurman K.
ASSISTANT EXAMINER: Kishori, G. S.
LEGAL REPRESENTATIVE: Hamilton, Brook, Smith & Reynolds
NUMBER OF CLAIMS: 30
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 5 Drawing Figure(s); 3 Drawing Page(s)
LINE COUNT: 807
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention pertains to a method for immobilizing proteins or peptides onto a flat, microporous membrane surface in a form suitable for sequence analysis or other chemical or enzymatic processes. The process involves the formation of a thin polymer network that entraps the protein or peptide therein.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

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L28           21 L5 NOT L25

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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 19 Jan 2006 (20060119/PD)
FILE LAST UPDATED: 19 Jan 2006 (20060119/ED)
HIGHEST GRANTED PATENT NUMBER: US6988280
HIGHEST APPLICATION PUBLICATION NUMBER: US2006015978
CA INDEXING IS CURRENT THROUGH 19 Jan 2006 (20060119/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 19 Jan 2006 (20060119/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2005


=> d que nos L7
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L2              STR
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L7           13 SEA FILE=USPATFULL ABB=ON  PLU=ON  L4


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L29           3 L7 NOT L26

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L30           25 DUP REM L28 L23 L29 L9 (6 DUPLICATES REMOVED)
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                 ANSWERS '22-24' FROM FILE USPATFULL
                 ANSWER '25' FROM FILE CHEMCATS

=> d ibib abs hitind hitstr L30 1-21; d ibib abs hitstr L30 22-24; d iall L30 25

L30  ANSWER 1 OF 25  CAPLUS  COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2005:105992  CAPLUS
DOCUMENT NUMBER:          142:331952
TITLE:                    Synthesis and biodistribution of [11C]R116301, a
                          promising PET ligand for central NK1 receptors
AUTHOR(S):                Van der Mey, M.; Janssen, C. G. M.; Janssens, F. E.;
                          Jurzak, M.; Langlois, X.; Sommen, F. M.; Verreet, B.;
                          Windhorst, A. D.; Leysen, J. E.; Herscheid, J. D. M.
CORPORATE SOURCE:         Location Radionuclide Center, Department of Nuclear
                          Medicine and PET Research, VU University Medical
                          Center, Amsterdam, 1081 HV, Neth.
SOURCE:                   Bioorganic & Medicinal Chemistry (2005), 13(5),
                          1579-1586
                          CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER:                Elsevier Ltd.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 142:331952
AB   N1-(2,6-Dimethylphenyl)-2-(4-{(2R,4S)-2-benzyl-1-[3,5-
     di(trifluoromethyl)[carbonyl-11C]benzoyl]hexahydro-4-
     pyridinyl}piperazino)acetamide ([11C]R116301) was prepared and evaluated as
```

a potential positron emission tomog. (PET) ligand for investigation of central neurokinin(1) (NK1) receptors. 1-Bromo-3,5-di(trifluoromethyl)benzene was converted in three steps into 3,5-di(trifluoromethyl)[carbonyl-11C]benzoyl chloride, which was reacted with N1-(2,6-dimethylphenyl)-2-{4-[(2R,4S)-2-benzylhexahydro-4-pyridinyl]piperazino}acetamide providing [11C]R116301 in 45-57% decay-corrected radiochem. yield. The total synthesis time, from end of bombardment (EOB) to the formulated product, was 35 min. Specific activity (SA) was 82-172 GBq/μmol (n = 10) at the end of synthesis. N1-([4-3H]-2,6-Dimethylphenyl)-2-(4-{(2R,4S)-2-benzyl-1-[3,5-di(trifluoromethyl)benzoyl]hexahydro-4-pyridinyl}piperazino)acetamide ([3H]R116301) was also synthesized (SA: 467 GBq/mmol). The Bmax for [3H]R116301 measured in vitro on Chinese hamster ovary cell membranes stably transfected with the human NK1 receptor was 19.10 ± 1.02 pmol/mg protein with an apparent dissociation constant of 0.08 ± 0.01 nM. Ex vivo, in vivo and in vitro autoradiog. studies with [3H]R116301 in gerbils demonstrated a preferential accumulation of the radioactivity in the striatum, olfactory tubercule, olfactory bulb and locus coeruleus. In vivo, the biodistribution of [11C]R116301 in gerbils revealed that the highest initial uptake is in the lung, followed by the liver and kidney. In the brain, maximum accumulation was found in the olfactory tubercules (1.10 ± 0.08 injected dose (ID)/g 20 min post injection (p.i.)) and the nucleus accumbens (1.00 ± 0.12 ID/g 10 min p.i.). Tissue/cerebellum concentration ratios for striatum and nucleus accumbens increased with time due to rapid uptake followed by a slow wash out (1.29 and 1.64, resp., 30 min p.i.). A tissue to cerebellum ratio of 1.33 and 1.62 was also observed for olfactory bulb and olfactory tubercules, resp. (20 min p.i.). In summary, [11C]R116301 appears to be a promising radioligand suitable for the visualization of NK1 receptors in vivo using PET.

CC 8-9 (Radiation Biochemistry)

IT **848440-93-7P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biodistribution of [11C]R116301, a promising PET ligand for central NK1 receptors)

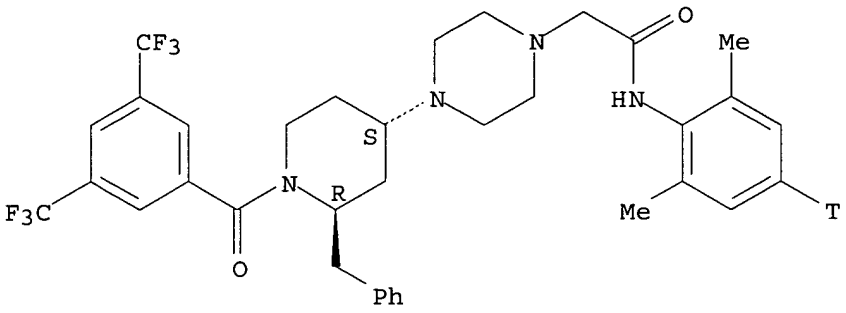
IT **848440-91-5P**
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and biodistribution of [11C]R116301, a promising PET ligand for central NK1 receptors)

IT **848440-93-7P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biodistribution of [11C]R116301, a promising PET ligand for central NK1 receptors)

RN 848440-93-7 CAPLUS

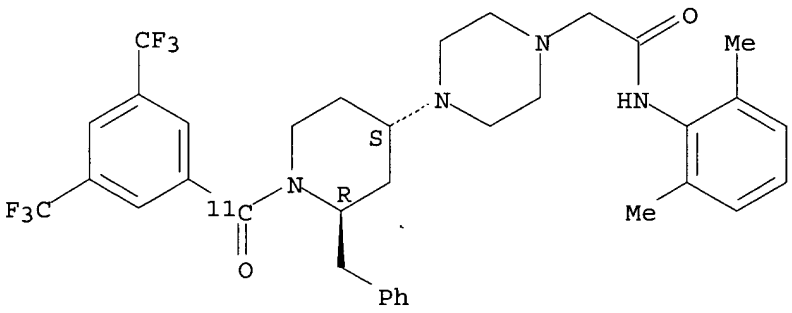
CN 1-Piperazineacetamide, 4-[(2R,4S)-1-[3,5-bis(trifluoromethyl)benzoyl]-2-(phenylmethyl)-4-piperidinyl]-N-(2,6-dimethylphenyl-4-t)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **848440-91-5P**
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and biodistribution of [11C]R116301, a promising PET ligand for central NK1 receptors)
RN 848440-91-5 CAPLUS
CN 1-Piperazineacetamide, 4-[(2R,4S)-1-[3,5-bis(trifluoromethyl)benzoyl-carbonyl-11C]-2-(phenylmethyl)-4-piperidinyl]-N-(2,6-dimethylphenyl)-(9CI) (CA INDEX NAME)

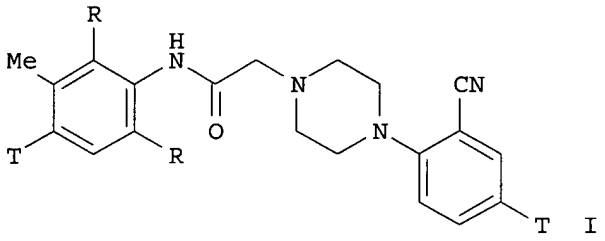
Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2004:767283 CAPLUS
DOCUMENT NUMBER: 141:410897
TITLE: Synthesis and activity of 2-[4-(4-[3H]-2-cyanophenyl)piperazinyl]-N-(2,4,6-[3H]3-3-methylphenyl)acetamide: a selective dopamine D4 receptor agonist and radioligand
AUTHOR(S): Matulenko, Mark A.; Surber, Bruce; Fan, Leimin; Kolasa, Teodozyi; Nakane, Masaki; Terranova, Marc A.; Uchic, Marie E.; Miller, Loan N.; Chang, Renjie; Donnelly-Roberts, Diana L.; Namovic, Marian T.; Moreland, Robert B.; Brioni, Jorge D.; Stewart, Andrew O.
CORPORATE SOURCE: Neuroscience Research, Global Pharmaceutical Research and Development, AP9A/L16, Abbott Laboratories, Abbott Park, IL, 60064-6115, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(20), 5095-5098

CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:410897
GI



I

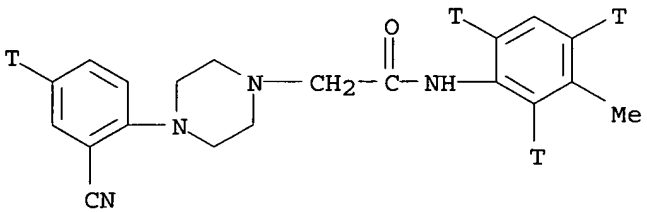
AB The first selective dopamine D4 agonist radioligand I [R = H, T] is described. The synthesis of I relied on the transformation of brominated precursors with tritium gas in the presence of a sensitive cyano functional group. The specific activity of I was measured and I [R = T] found to be suitable for use in D4 saturation and competition binding studies. The synthesis, biol., and radioactivity of this new agonist radioligand as well as preliminary SAR is discussed.

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

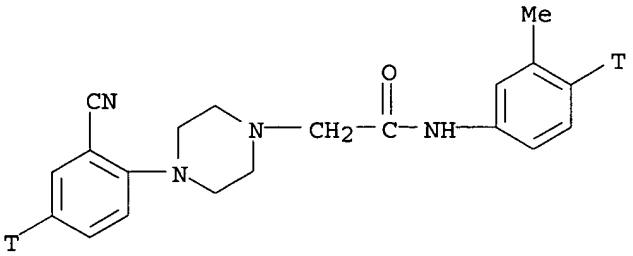
IT 630116-03-9P **741701-47-3P 791846-36-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of tritiated 2-[4-(4-[3H]-2-cyanophenyl)piperazinyl]-N-(2,4,6-[3H]3-3-methylphenyl)acetamide as a selective dopamine D4 receptor agonist and radioligand)

IT **741701-47-3P 791846-36-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of tritiated 2-[4-(4-[3H]-2-cyanophenyl)piperazinyl]-N-(2,4,6-[3H]3-3-methylphenyl)acetamide as a selective dopamine D4 receptor agonist and radioligand)

RN 741701-47-3 CAPLUS
CN 1-Piperazineacetamide, 4-(2-cyanophenyl-4-t)-N-(3-methylphenyl-2,4,6-t3)- (9CI) (CA INDEX NAME)



RN 791846-36-1 CAPLUS
CN 1-Piperazineacetamide, 4-(2-cyanophenyl-4-t)-N-(3-methylphenyl-4-t)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2001:665984 CAPLUS
DOCUMENT NUMBER: 136:6092
TITLE: Aqueous one-pot synthesis of derivatized cyclopentadienyl-tricarbonyl complexes of 99mTc with an in situ CO source: Application to a serotonergic receptor ligand
AUTHOR(S): Wald, Joachim; Alberto, Roger; Ortner, Kirstin; Candreia, Lukas
CORPORATE SOURCE: Institute of Inorganic Chemistry, University of Zurich, Zurich, 8057, Switz.
SOURCE: Angewandte Chemie, International Edition (2001), 40(16), 3062-3066
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:6092

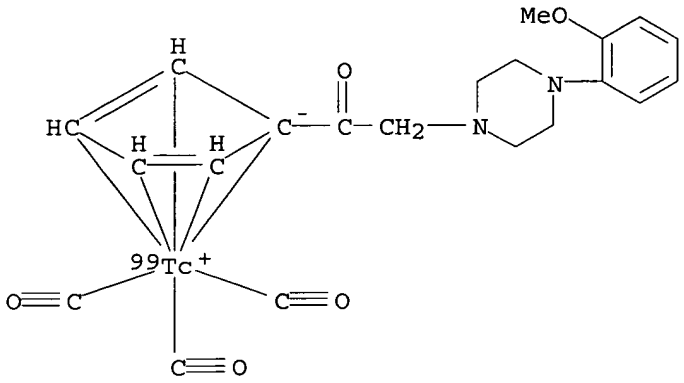
AB The authors demonstrated that half-sandwich complexes [(RCp)M(CO)3] (M = Re, 99mTc; R = MeCO, PhCO, o-MeOC6H4QCH2CO (Q = piperazine-1,4-diyl)) can easily be synthesized if the acid dissociation constant of the cyclopentadiene ring is increased. E.g., the reaction of acetylcyclopentadiene and derivs. with fac-[99mTc(OH2)3(CO)3]+ directly yielded the radiopharmaceutically relevant complexes [(RCp)99mTc(CO)3] (R = MeCO, o-MeOC6H4QCH2CO (Q = piperazine-1,4-diyl)) in good yields. The major impact of this work emerges from the general possibility of introducing the very small and highly lipophilic [Cp99mTc(CO)3] moiety in a wide variety of small receptor-binding biomols. Also the direct reaction of acidic and water-soluble cyclopentadiene compds. with aqua ions could lead to interesting and novel species in aqueous organometallic chemical The prepared rhenium compds. (RCp)Re(CO)3 (R = PhCO (9), o-MeOC6H4QCH2CO (Q = piperazine-1,4-diyl) (10)) were crystallized and their structures were elucidated by x-ray studies.

CC 29-11 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 8, 63, 75, 78

IT 12266-77-2P, (η5-Acetylcyclopentadienyl)tricarbonylrhenium
139410-50-7P, Tricarbonyl(η5-acetylcyclopentadienyl)technetium-99Tc
374929-96-1P **374929-97-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **374929-97-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 374929-97-2 CAPLUS
CN Technetium-99Tc, tricarbonyl[(1,2,3,4,5-η)-1-[[4-(2-methoxyphenyl)-1-piperazinyl]acetyl]-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2002:174788 CAPLUS
DOCUMENT NUMBER: 137:370047
TITLE: The preparation of isotopically labeled 2,4,6-trisubstituted pyrimidines
AUTHOR(S): Stolle, W. T.; Hsi, R. S. P.; Easter, J. A.
CORPORATE SOURCE: Pharmacia Corporation, Kalamazoo, MI, USA
SOURCE: Synthesis and Applications of Isotopically Labelled Compounds, Proceedings of the International Symposium, 7th, Dresden, Germany, June 18-22, 2000 (2001), Meeting Date 2000, 272-275. Editor(s): Pleiss, Ulrich; Voges, Rolf. John Wiley & Sons Ltd.: Chichester, UK.
CODEN: 69CIJC; ISBN: 0-471-49501-8
DOCUMENT TYPE: Conference
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:370047
AB The condensation reactions involving isotopically labeled urea or thiourea with di-Et malonate or Et cyanoacetate were successfully used to synthesize the core structural component, 2,4,6-trisubstituted pyrimidines, for several pharmaceutical candidates. Three case studies are presented, involving tirilazad mesylate, pyrrolopyrimidine, and a non-nucleoside reverse transcriptase inhibitor, which were chosen for drug development requiring the preparation of radioisotope and/or stable isotope labeled material for drug absorption, distribution, metabolism, and excretion (ADME) studies. The resulting labeled pyrimidines exhibited excellent metabolic stability when used for clin. and pre-clin. ADME studies.
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **161860-82-8P** 475292-29-6P 475292-33-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically labeled 2,4,6-trisubstituted pyrimidines)
IT **161860-82-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically labeled 2,4,6-trisubstituted pyrimidines)
RN 161860-82-8 CAPLUS

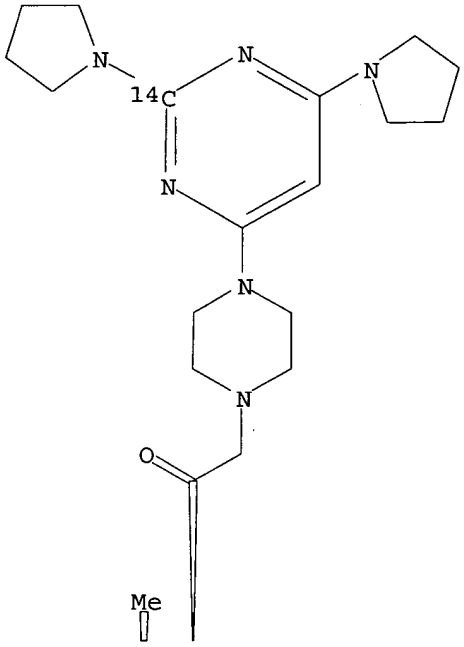
CN Pregna-1,4,9(11)-triene-3,20-dione, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl-2-14C)-1-piperazinyl]-16-methyl-, (16α)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

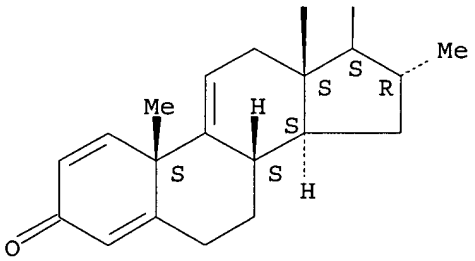
CRN 161860-81-7
CMF C38 H52 N6 O2

Absolute stereochemistry.

PAGE 1-A

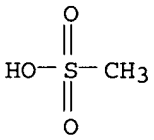


PAGE 2-A



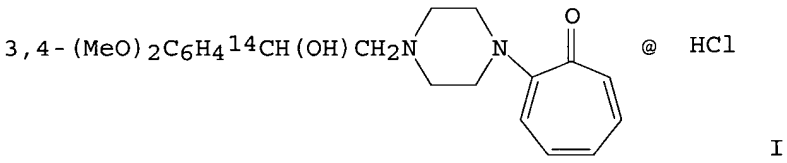
CM 2

CRN 75-75-2
CMF C H4 O3 S



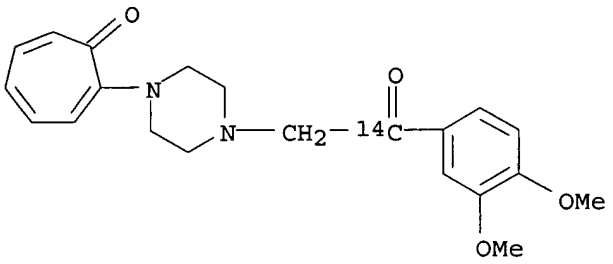
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 1989:423479 CAPLUS
DOCUMENT NUMBER: 111:23479
TITLE: Synthesis of [carbon-14]ciladopa
AUTHOR(S): Hicks, D. R.; Dolak, L.; Foss, D.
CORPORATE SOURCE: Dep. Biochem., Ayerst Lab. Res., Inc., Princeton, NJ, 08543, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1988), 25(12), 1307-13
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:23479
GI

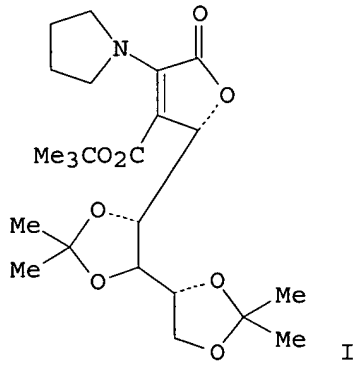


I

AB [14C]Ciladopa, (S)-(-)-2-[4-[[2-14C]-2-hydroxy-2-(3,4-dimethoxyphenyl)ethyl]-1-piperazinyl]-2,4,6-cycloheptatrien-1-one hydrochloride (I), was synthesized in six steps incorporating [14C]carbon dioxide. [7-14C]acetoveratrole, 3,4-(MeO)2C6H414COMe, obtained from veratric acid via the acid chloride, was brominated and coupled with a troponylpiperazine salt. The resulting ketone was stereospecifically reduced microbiol. to give the (S)-(-) enantiomer of the alc. Two batches of I were produced, giving a combined overall yield of 25% from [14C]barium carbonate (sp. act. 44.7 ± 0.6 and 43.4 ± 0.8 μCi/mg; 99.2 and 98.9% radiochem. purity, resp.).
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 9
IT **121163-53-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and enzymic reduction of, by Candida guilliermondii)
IT **121163-53-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and enzymic reduction of, by Candida guilliermondii)
RN 121163-53-9 CAPLUS
CN 2,4,6-Cycloheptatrien-1-one, 2-[4-[2-(3,4-dimethoxyphenyl)-2-oxoethyl-2-14C]-1-piperazinyl]- (9CI) (CA INDEX NAME)



L30 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 1987:637184 CAPLUS
DOCUMENT NUMBER: 107:237184
TITLE: Vinyl carbanions. Part 30. A convenient synthesis of 3-deoxy-D-gluco-2-octulosonate (D-gluco KDO)
AUTHOR(S): Lafont, Dominique; Hoch, Monika; Schmidt, Richard R.
CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: Journal of Carbohydrate Chemistry (1986), 5(4), 601-14
CODEN: JCACDM; ISSN: 0732-8303
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:237184
GI



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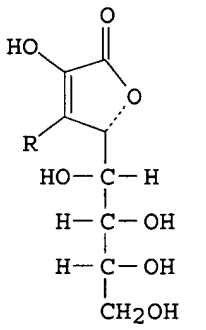
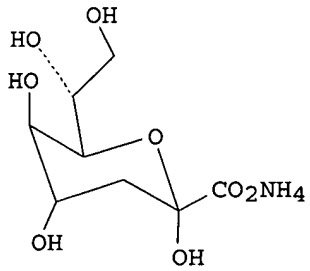


II



III

AB Treatment of di-tert-butyl (E)-2-(1-pyrrolidinyl)-2-butenedioate with Li diisopropylamide in THF followed by treatment with 2,3:4,5-di-O-isopropylidene-D-arabinose gave 44% gluco-octenolactone I and 11% manno isomer. I dissolved in MeOH-H2O was treated with CF3CO2H to give 60% lactone II (R = CO2CMe3), which on heating in H2O gave 74% II (R = H), which on treatment with NH3 gave D-gluco-KDO salt III.

CC 33-8 (Carbohydrates)

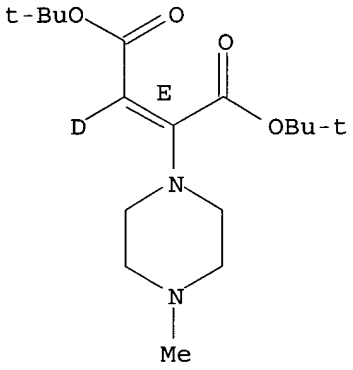
IT 20603-27-4P 87949-30-2P 111375-94-1P 111375-99-6P
111376-00-2P 111376-01-3P 111376-02-4P 111376-03-5P
111376-09-1P 111376-11-5P 111376-12-6P 111376-13-7P 111554-16-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **111376-00-2P 111376-01-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 111376-00-2 CAPLUS

CN 2-Butenedioic-2-d acid, 3-(4-methyl-1-piperazinyl)-, bis(1,1-dimethylethyl) ester, (E)- (9CI) (CA INDEX NAME)

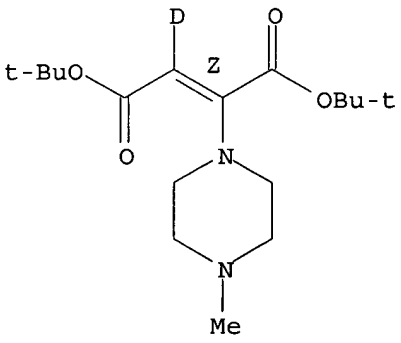
Double bond geometry as shown.



RN 111376-01-3 CAPLUS

CN 2-Butenedioic-2-d acid, 3-(4-methyl-1-piperazinyl)-, bis(1,1-dimethylethyl) ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



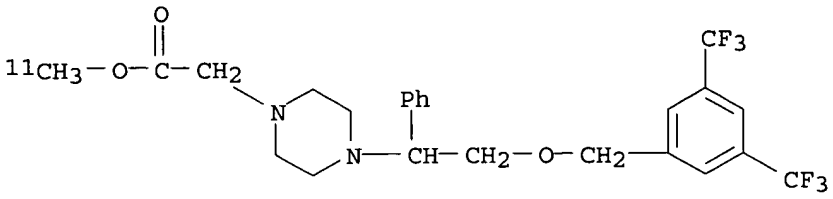
L30 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:581586 CAPLUS

DOCUMENT NUMBER: 143:281735
TITLE: Synthesis and initial PET imaging of new potential NK1 receptor radioligands 1-[2-(3,5-bis-trifluoromethyl-benzyloxy)-1-phenyl-ethyl]-4-[11C]methyl-piperazine and {4-[2-(3,5-bis-trifluoromethyl-benzyloxy)-1-phenyl-ethyl]-piperazine-1-yl}-acetic acid [11C]methyl ester
AUTHOR(S): Gao, Mingzhang; Mock, Bruce H.; Hutchins, Gary D.; Zheng, Qi-Huang
CORPORATE SOURCE: Department of Radiology, Indiana University School of Medicine, Indianapolis, IN, 46202-2111, USA
SOURCE: Nuclear Medicine and Biology (2005), 32(5), 543-552
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The NK1 receptor radioligands 1-[2-(3,5-bis-trifluoromethyl-benzyloxy)-1-phenyl-ethyl]-4-[11C]methyl-piperazine ([11C]BMP, [11C]1) and {4-[2-(3,5-bis-trifluoromethyl-benzyloxy)-1-phenyl-ethyl]-piperazine-1-yl}-acetic acid [11C]methyl ester ([11C]BME, [11C]2) were synthesized for evaluation as new potential PET imaging agents for brain NK1 receptors. The new tracers [11C]BMP and [11C]BME were prepared by N-[11C]methylation and O-[11C]methylation of corresponding precursors 1-[2-(3,5-bis-trifluoromethyl-benzyloxy)-1-phenyl-ethyl]-piperazine and {4-[2-(3,5-bis-trifluoromethyl-benzyloxy)-1-phenyl-ethyl]-piperazine-1-yl}-acetic acid using [11C]methyl triflate and isolated by solid-phase extraction (SPE) purification procedure with 40-55% radiochem. yields, decay corrected to end of bombardment, and a synthesis time of 15-20 min. The initial PET dynamic studies of the tracers [11C]1 and [11C]2 in rats were performed using an animal PET scanner, IndyPET-II, developed in our laboratory The results show the tracer [11C]BMP had better uptake in the animal brain than the tracer [11C]BME and gave higher quality rat brain images. Blocking studies by i.v. coinjection of hot tracer [11C]BMP with cold drug BMP had no effect on [11C]BMP-PET rat brain imaging. Likewise, blocking studies by i.v. coinjection of hot tracer [11C]BME with cold drug BME also showed no effect on [11C]BME-PET rat brain imaging. These results suggest that the localization of [11C]BMP and [11C]BME in rat brain is mediated by nonspecific processes, and the visualization of [11C]BMP-PET and [11C]BME-PET on rat brain is related to nonspecific binding.

CC 8-9 (Radiation Biochemistry)
IT 864464-58-4P **864464-59-5P**
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and initial PET imaging of new potential NK1 receptor radioligands [11C]BMP and [11C]BME)
IT **864464-59-5P**
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and initial PET imaging of new potential NK1 receptor radioligands [11C]BMP and [11C]BME)
RN 864464-59-5 CAPLUS
CN 1-Piperazineacetic acid, 4-[2-[[3,5-bis(trifluoromethyl)phenyl]methoxy]-1-phenylethyl]-, methyl-11C ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:674075 CAPLUS
DOCUMENT NUMBER: 141:200544
TITLE: [3H] A-369508 (2-[4-(2-cyanophenyl)-1-piperazinyl]-N-(3-methylphenyl) acetamide): an agonist radioligand selective for the dopamine D4 receptor
AUTHOR(S): Moreland, Robert B.; Terranova, Marc A.; Chang, Renjie; Uchic, Marie E.; Matulenko, Mark A.; Surber, Bruce W.; Stewart, Andrew O.; Brioni, Jorge D.
CORPORATE SOURCE: Neuroscience Research Global Pharmaceutical Research and Development, Abbott Laboratories, Abbott Park, IL, 60064-6118, USA
SOURCE: European Journal of Pharmacology (2004), 497(2), 147-154
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

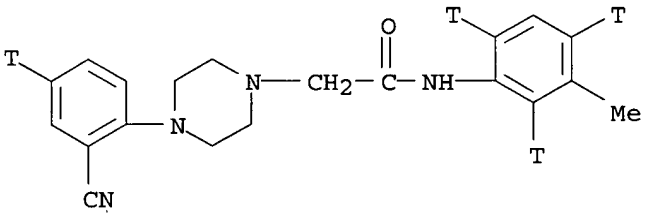
AB Tritiation of the dopamine D4 receptor selective agonist A-369508 (2-[4-(2-cyanophenyl)-1-piperazinyl]-N-(3-methylphenyl) acetamide) has provided a radioligand for the characterization of dopamine D4 receptors. [3H] A-369508 binds with high affinity to the major human dopamine D4 receptor variants D4.2, D4.4 and D4.7 (Kd=1.7, 4, and 1.2 nM, resp.). It also binds to the rat dopamine D4 receptor, (Kd=4.4 nM), implying similar binding affinity across human and rat receptors. A-369508 shows >400-fold selectivity over D2L, >350-fold selectivity over 5-HT1A and >700-1000-fold selectivity over all other receptors tested. Agonist activity determined by inhibition of forskolin-induced cAMP in Chinese hamster ovary cells transfected with the human dopamine D4.4 receptor (EC50=7.5 nM, intrinsic activity=0.71) indicates that A-369508 is a potent agonist at the human dopamine D4 receptor. Similar data was observed in other functional assays. [3H] A-369508 binds to a single, high affinity site on membranes containing the human dopamine D4.4 receptor. When compared to the D2-like antagonist [3H] spiperone, competition binding for agonists like dopamine and apomorphine were 2-10-fold more potent with [3H] A-369508, while the antagonists clozapine, haloperidol and L-745870 bind with similar affinity to both ligands. Binding to rat brain regions demonstrated that the most abundant area was cerebral cortex (51.2 fmol/mg protein) followed by hypothalamus, hippocampus, striatum and cerebellum. [3H] A-369508 is a useful tool to define the localization and physiol. role of dopamine D4 receptors in central nervous system and can facilitate measuring accurate affinities (Ki) for structure/activity relationship studies designed to identify dopamine D4 receptor selective agonists.

CC 2-8 (Mammalian Hormones)
Section cross-reference(s): 1
IT 630116-03-9, A 369508 **741701-47-3**, [3H]-A 369508
RL: BSU (Biological study, unclassified); BUU (Biological use,

unclassified); BIOL (Biological study); USES (Uses)
([3H] A-369508 (2-[4-(2-cyanophenyl)-1-piperazinyl]-N-(3-methylphenyl) acetamide), an agonist radioligand selective for dopamine D4 receptor)

IT **741701-47-3**, [3H]-A 369508
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
([3H] A-369508 (2-[4-(2-cyanophenyl)-1-piperazinyl]-N-(3-methylphenyl) acetamide), an agonist radioligand selective for dopamine D4 receptor)

RN 741701-47-3 CAPLUS
CN 1-Piperazineacetamide, 4-(2-cyanophenyl-4-t)-N-(3-methylphenyl-2,4,6-t3)-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:376987 CAPLUS
DOCUMENT NUMBER: 138:385215
TITLE: Preparation of isotopically-coded affinity markers for mass spectrometric analysis of proteins
INVENTOR(S): Lerchen, Hans-Georg; Siegmund, Hans-Ulrich; Immler, Dorian; Schumacher, Andreas; Auriel, Daniel
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003040288	A2	20030515	WO 2002-EP12105	20021030
WO 2003040288	A3	20031211		
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EP 1446665	A2	20040818	EP 2002-774759	20021030
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EP 1477493 A1 20041117 EP 2003-9894 20030515
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US 2005049406 A1 20050303 US 2004-494999 20041029
PRIORITY APPLN. INFO.: DE 2001-10154745 A 20011109
DE 2002-10234415 A 20020729
WO 2002-EP12105 W 20021030
OTHER SOURCE(S): MARPAT 138:385215
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention concerns isotopically-coded affinity markers (ICAT), A-L-PRG, e.g., I [A = affinity ligand (especially biotin); PRG = protein reactive group (maleimido, chloroalkyl, acryloyl); L = linker, L*; Z = NHCH2CO; L' = bridge between piperazines; R, R' = piperazine ring, D-, L- or (±)-amino acid; Z' = COCH2NH; k, l, m, n = 0 - 10, whereby k + l + m + n = 1 - 40] or its salts, for mass spectrometric anal. of proteins, and the preparation and use of said markers. Thus, biotin derivative I was prepared from piperazide II via regioselective deprotection, N-acylation with 3-maleimidopropionic acid, N-deprotection and coupling of, with biotin derivative III. Mass spectrometric anal. of proteins was carried out using ICAT I.

IC ICM C12N

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 9, 34

IT 525583-79-3P 525587-33-1P 525587-35-3P, N-Boc-[1,2-13C2]-Glycine methyl ester 525587-39-7P 525587-45-5P 525587-46-6P 525587-49-9P
525587-52-4P 525587-54-6P 525587-55-7P 525587-56-8P 525587-58-0P
525587-60-4P 525587-62-6P 525587-64-8P 525587-66-0P
525587-68-2P 525587-70-6P 525587-72-8P
525587-74-0P 525587-80-8P 525587-82-0P 525587-84-2P 525587-86-4P
525587-89-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and N-deprotection of; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-57-9P 525587-59-1P 525587-61-5P 525587-63-7P 525587-65-9P
525587-67-1P **525587-69-3P 525587-71-7P**
525587-73-9P 525587-83-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with biotin derivative; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-21-7P 525587-22-8P 525587-23-9P **525587-28-4P**
525587-30-8P 525587-32-0P 525587-51-3P 525587-81-9P
525587-95-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with biotin derivative; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

IT 525587-03-5P 525587-18-2P **525587-24-0P 525587-25-1P**
525587-26-2P 525587-34-2P 525587-44-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and regioselective N-deprotection of; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

IT 525586-41-8P 525586-42-9P 525586-43-0P 525586-44-1P 525586-45-2P
525586-46-3P 525586-47-4P 525586-48-5P 525586-49-6P 525586-50-9P
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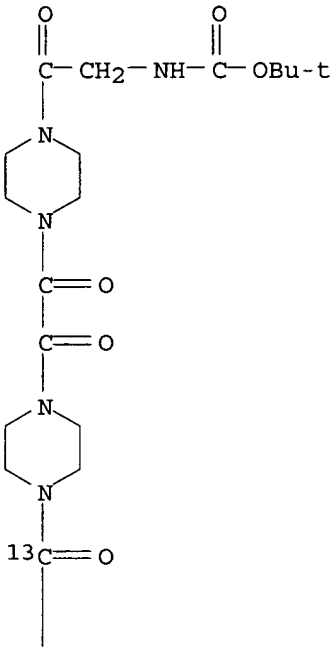
525586-72-5P 525586-73-6P 525586-74-7P 525586-75-8P 525586-76-9P
525586-77-0P 525586-78-1P **525586-79-2P 525586-80-5P**
525586-81-6P 525586-82-7DP, NovaSyn TG resin-bound amide
525586-83-8P 525586-84-9P 525586-85-0P 525586-86-1P 525586-87-2P
525586-88-3DP, aminopropylated silica gel-bound amide
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

IT **525587-68-2P 525587-70-6P 525587-72-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and N-deprotection of; preparation of isotopically-coded affinity
markers for mass spectrometric anal. of proteins)

RN 525587-68-2 CAPLUS

CN Carbamic acid, [2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]oxoacetyl]-1-piperazinyl]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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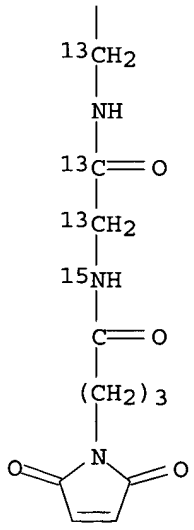

RN 525587-70-6 CAPLUS
CN Carbamic acid, [2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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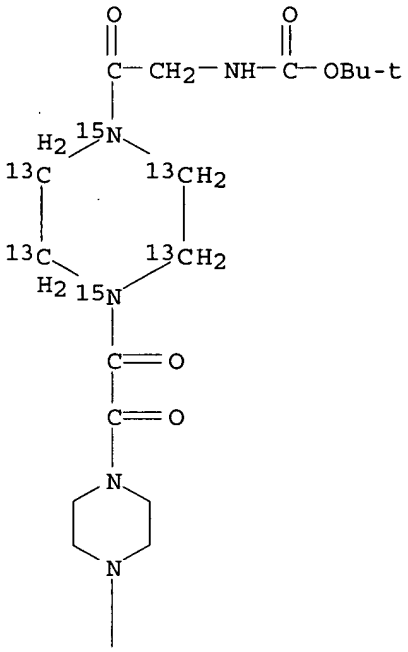

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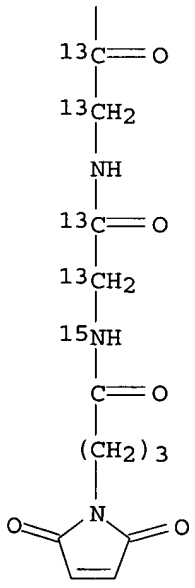
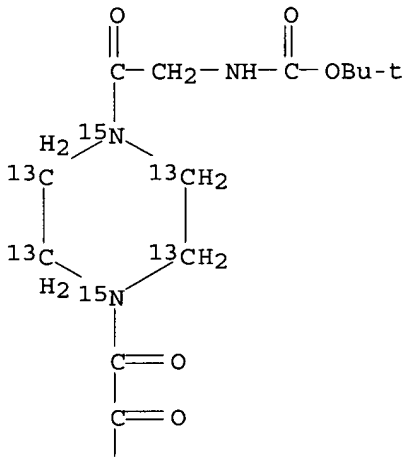


RN 525587-72-8 CAPLUS
CN Carbamic acid, [2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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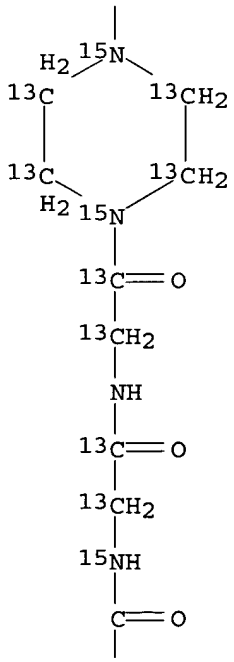

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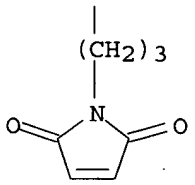
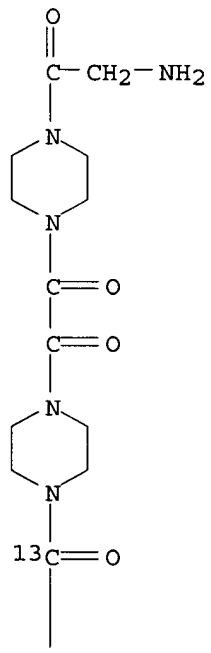


IT **525587-69-3P 525587-71-7P 525587-73-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with biotin derivative; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

RN 525587-69-3 CAPLUS

CN 1H-Pyrrole-1-butanamide-15N, N-[2-[[2-[4-[[4-(aminoacetyl)-1-piperazinyl]oxoacetyl]-1-piperazinyl]-2-oxoethyl-13C2]amino]-2-oxoethyl-13C2]-2,5-dihydro-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 1-A



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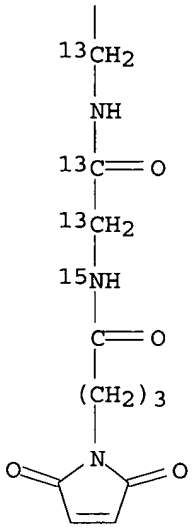
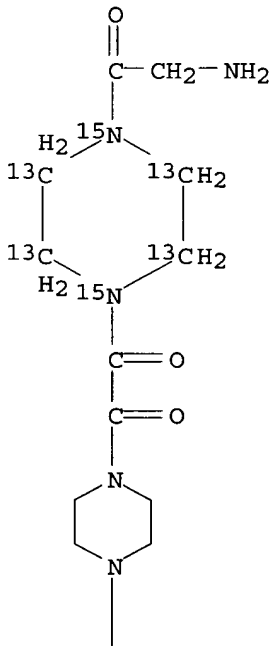


RN 525587-71-7 CAPLUS
CN 1H-Pyrrole-1-butanamide-15N, N-[2-[[2-[4-[[4-(aminoacetyl)-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]oxoacetyl]-1-piperazinyl]-2-oxoethyl-13C2]amino]-2-oxoethyl-13C2]-2,5-dihydro-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 1-A



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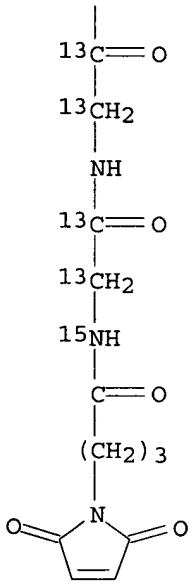
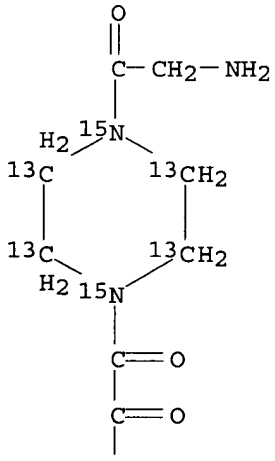


RN 525587-73-9 CAPLUS
CN 1H-Pyrrole-1-butanamide-15N, N-[2-[[2-[4-[[4-(aminoacetyl)-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl-13C2]amino]-2-oxoethyl-13C2]-2,5-dihydro-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 1-A



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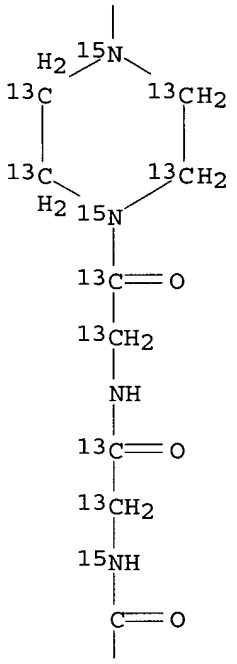

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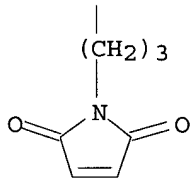

IT **525587-28-4P 525587-30-8P 525587-32-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with biotin derivative; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

RN 525587-28-4 CAPLUS

CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinylacetyl)-1-piperazinyl]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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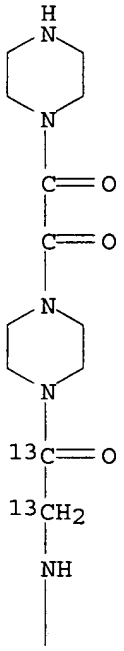
CRN 525587-27-3
CMF C22 H31 N7 O7

PAGE 1-A



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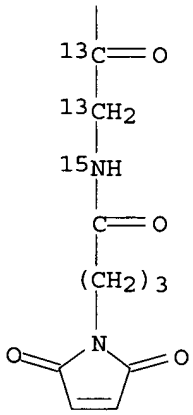
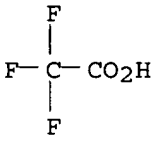


CM 2

CRN 76-05-1
CMF C2 H F3 O2

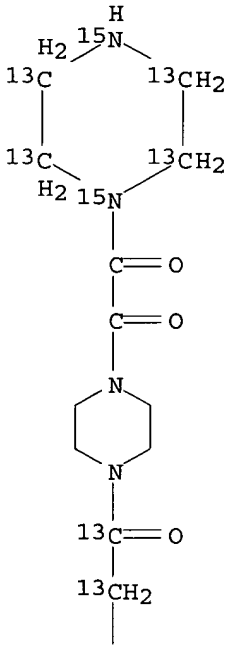


RN 525587-30-8 CAPLUS
CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-acetyl)-1-piperazinyl]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 525587-29-5
CMF C22 H31 N7 O7

PAGE 1-A



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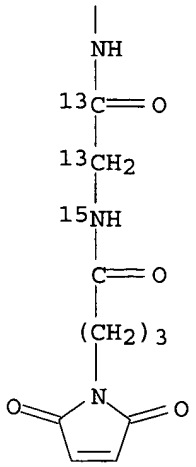
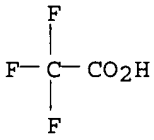


CM 2

CRN 76-05-1
CMF C2 H F3 O2

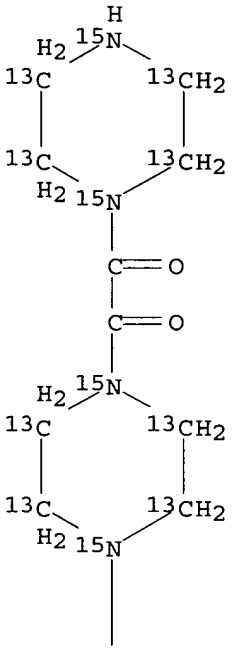


RN 525587-32-0 CAPLUS
CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-acetyl)-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 525587-31-9
CMF C22 H31 N7 O7

PAGE 1-A



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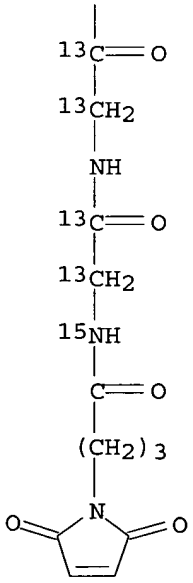
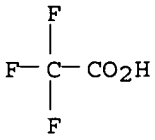


CM 2

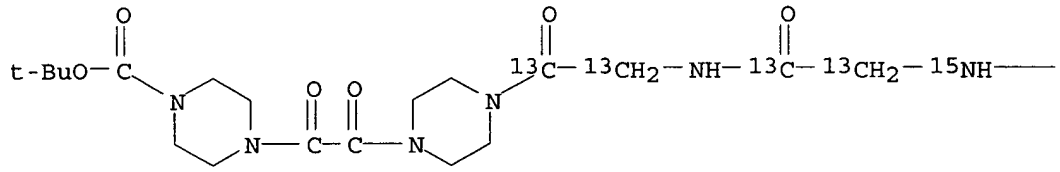
CRN 76-05-1
CMF C2 H F3 O2



IT **525587-24-0P 525587-25-1P 525587-26-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and regioselective N-deprotection of; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

RN 525587-24-0 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[oxo[4-[[[[[(phenylmethoxy)carbonyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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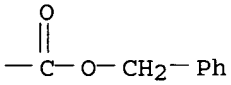
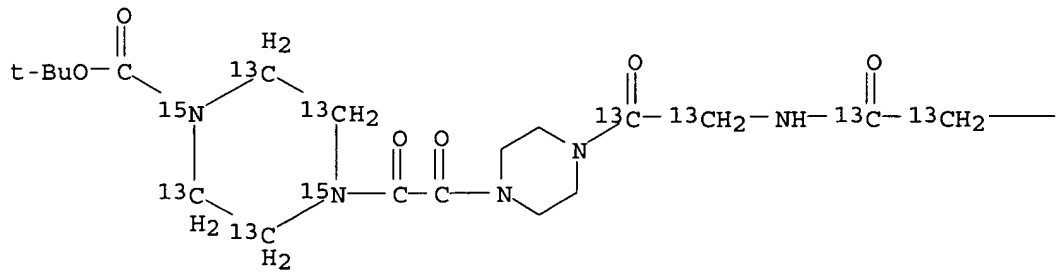


RN 525587-25-1 CAPLUS
CN 1-Piperazine-2,3,5,6-13C4-1,4-15N2-carboxylic acid, 4-[oxo[4-[[[[[(phenylmethoxy)carbonyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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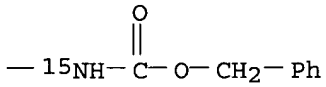
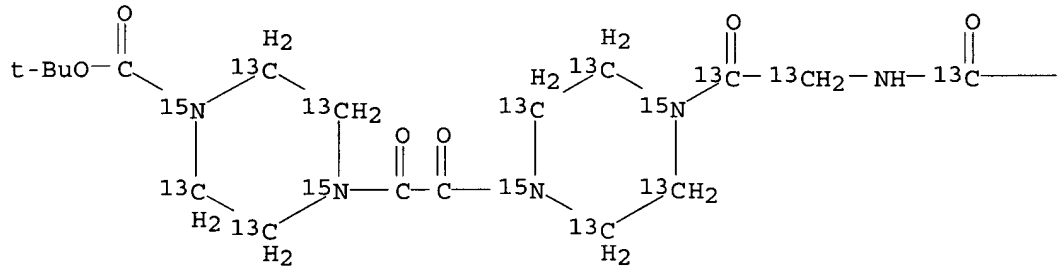


RN 525587-26-2 CAPLUS
CN 1-Piperazine-2,3,5,6-13C4-1,4-15N2-carboxylic acid, 4-[oxo[4-[[[[[(phenylmethoxy)carbonyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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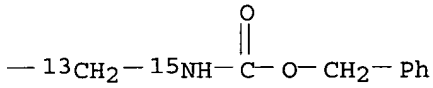
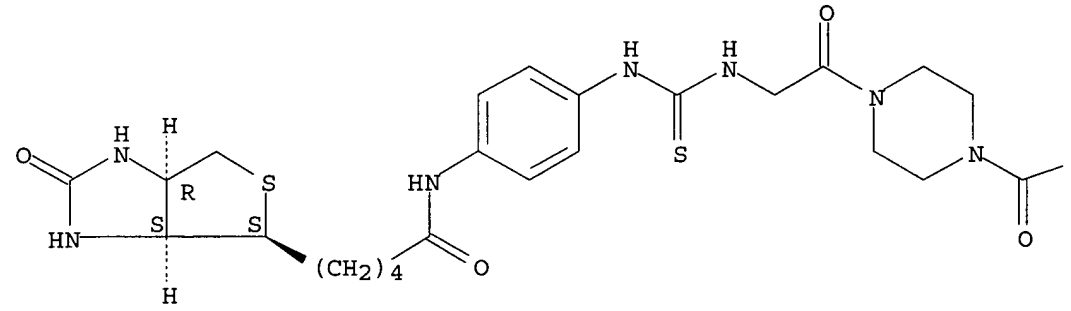


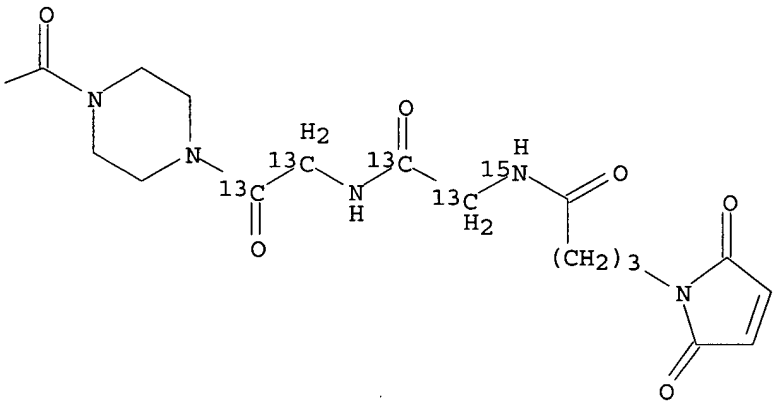
IT **525586-79-2P 525586-80-5P 525586-81-6P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)
RN 525586-79-2 CAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[4-[[[[2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]oxoacetyl]-1-piperazinyl]-2-oxoethyl]amino]thioxomethyl]amino]phenyl]hexahydro-2-oxo-, (3aS,4S,6aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



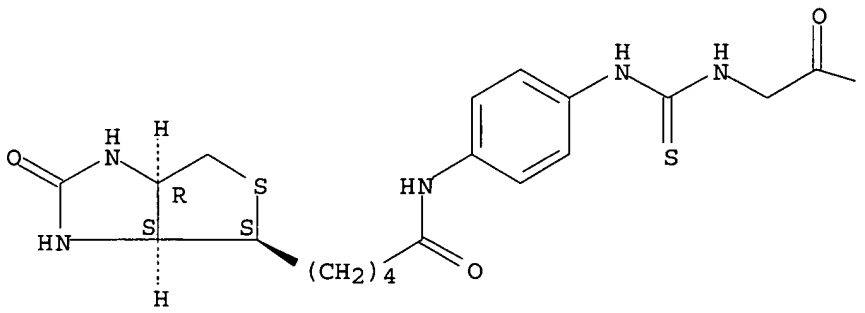
PAGE 1-B



RN 525586-80-5 CAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[4-[[[[2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl]amino]thioxomethyl]amino]phenyl]hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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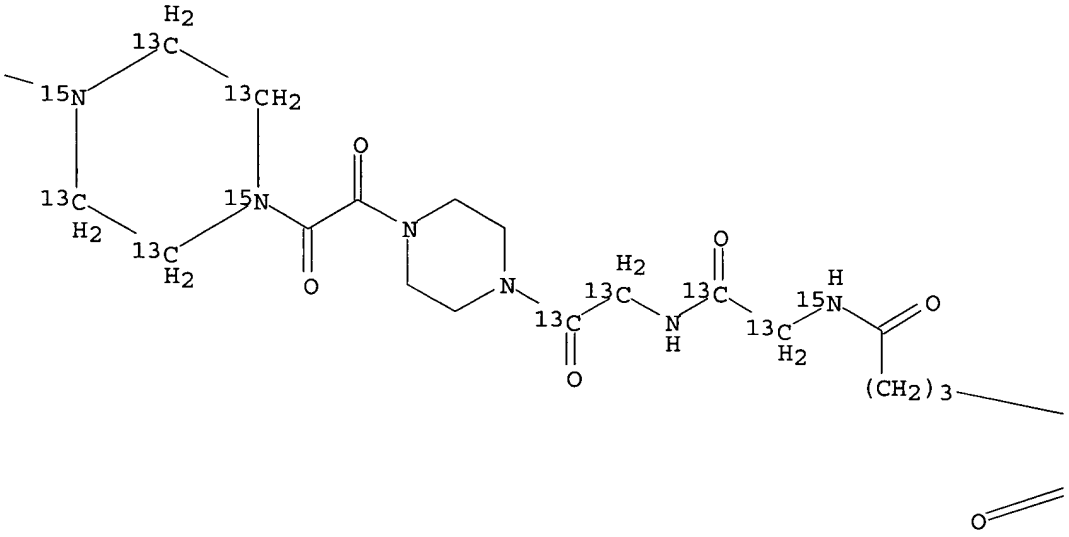

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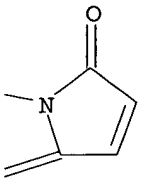
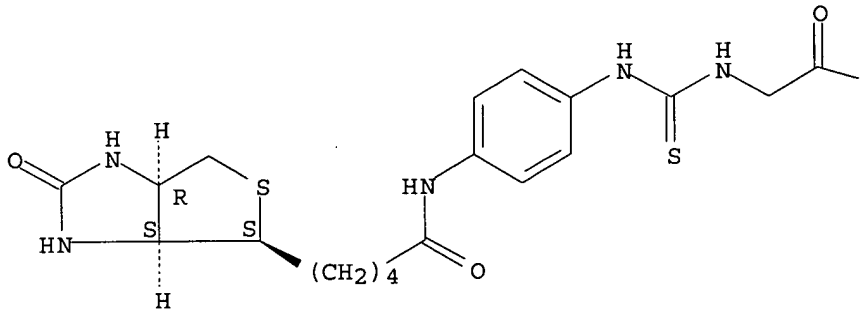


RN 525586-81-6 CAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[4-[[[[2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl]amino]thioxomethyl]amino]phenyl]hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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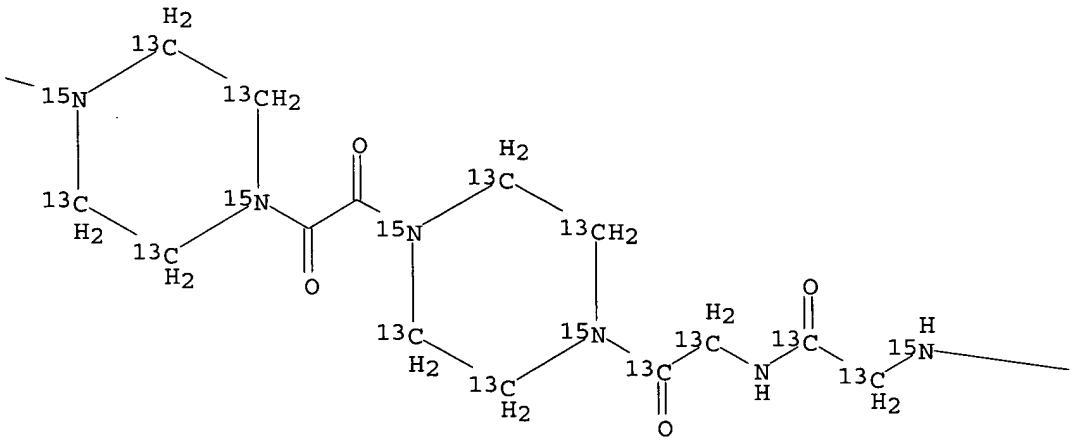
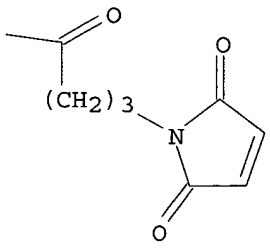




L30 ANSWER 10 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:725193 CAPLUS
DOCUMENT NUMBER: 139:32571
TITLE: Comparative distribution of binding of the muscarinic receptor ligands pirenzepine, AF-DX 384, (R,R)-I-QNB and (R,S)-I-QNB to human brain
AUTHOR(S): Piggott, Margaret; Owens, Jonathan; O'Brien, John; Paling, Sean; Wyper, David; Fenwick, John; Johnson, Mary; Perry, Robert; Perry, Elaine
CORPORATE SOURCE: Centre Development in Clinical Brain Ageing, MRC/University of Newcastle, Newcastle General Hospital, Newcastle-upon-Tyne, NE4 6BE, UK
SOURCE: Journal of Chemical Neuroanatomy (2002), 24(3), 211-223
CODEN: JCNAEE; ISSN: 0891-0618
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Quinuclidinyl benzilate (QNB) and its derivs. are being developed to investigate muscarinic receptor changes in vivo in Alzheimer's disease and dementia with Lewy bodies. This is the first study of [125I]-(R,R)-I-QNB and [125I]-(R,S)-I-QNB binding in vitro in human brain. We have compared the in vitro binding of the muscarinic ligands [3H]pirenzepine and [3H]AF-DX 384, which have selectivity for the M1 and M2/M4 receptor subtypes, resp., to the binding of [125I]-(R,R)-I-QNB and [125I]-(R,S)-I-QNB. This will provide a guide to the interpretation of in vivo SPET images generated with [123I]-(R,R)-I-QNB and [123I]-(R,S)-I-QNB. Binding was investigated in striatum, globus pallidus, thalamus and cerebellum, and cingulate, insula, temporal and occipital cortical areas, which show different proportions of muscarinic receptor subtypes, in post-mortem brain from normal individuals. M1 receptors are of high d. in cortex and striatum and are relatively low in the thalamus and cerebellum, while M4 receptors are mainly expressed in the striatum, and M2 receptors are most evident in the cerebellum and thalamus. [125I]-(R,R)-I-QNB and

[125I]-(R,S)-I-QNB d. distribution patterns were consistent with binding to both M1 and M4 receptors, with [125I]-(R,R)-I-QNB addnl. binding to a non-cholinergic site not displaceable by atropine. This distribution can be exploited by in vivo imaging, developing ligands for both SPET and PET, to reveal muscarinic receptor changes in Alzheimer's disease and dementia with Lewy bodies during the disease process and following cholinergic therapy.

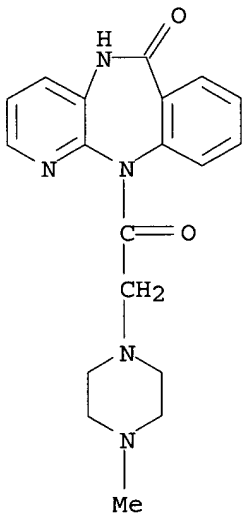
CC 8-9 (Radiation Biochemistry)

IT 88000-58-2 88000-63-9 **124620-97-9** 140186-38-5
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(comparative distribution of binding of the muscarinic receptor ligands pirenzepine, AF-DX 384, (R,R)-I-QNB and (R,S)-I-QNB to human brain)

IT **124620-97-9**
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
(comparative distribution of binding of the muscarinic receptor ligands pirenzepine, AF-DX 384, (R,R)-I-QNB and (R,S)-I-QNB to human brain)

RN 124620-97-9 CAPLUS

CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:675170 CAPLUS

DOCUMENT NUMBER: 138:122357

TITLE: Molecular structure, hydrogen bonding, basicity and spectroscopic properties of N,N'-dimethylpiperazine betaines and their hydrohalides

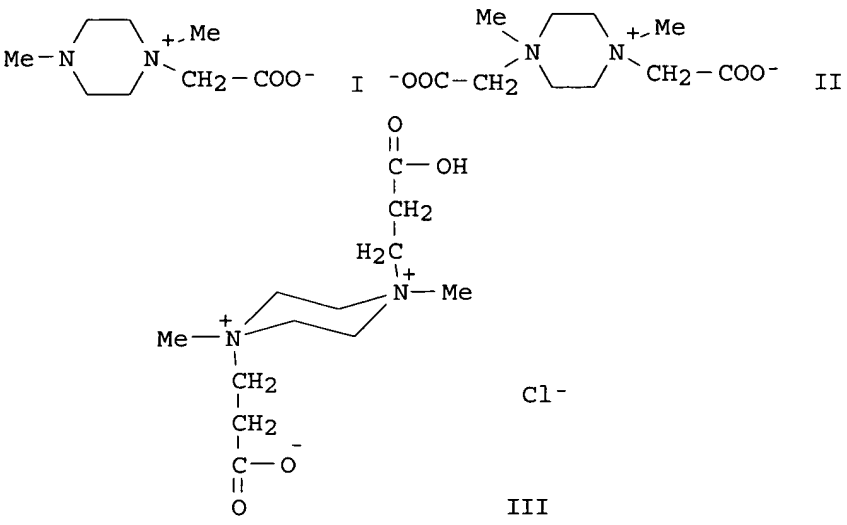
AUTHOR(S): Dega-Szafran, Z.; Jaskolski, M.; Kurzyca, I.; Barczynski, P.; Szafran, M.

CORPORATE SOURCE: Faculty of Chemistry, Adam Mickiewicz University, Poznan, 60-780, Pol.

SOURCE: Journal of Molecular Structure (2002), 614(1-3), 23-32
CODEN: JMOSB4; ISSN: 0022-2860

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal
LANGUAGE: English
GI



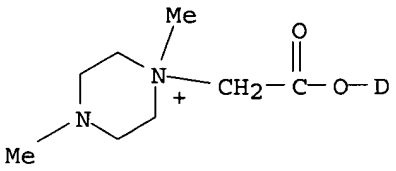
AB Two N,N'-dimethylpiperazine betaines [mono (I) and double (II)] have been synthesized. Betaine I reacts with two equivalent of HCl or HBr, while II only with one. In the crystal structure of N,N'-dicarboxymethyl-N,N'-dimethylpiperazine monohydrochloride (N,N'-dimethylpiperazine doublebetaine monohydrochloride, III) determined by X-ray diffraction, the piperazinium moieties form infinite chains bridged by very strong, sym. and linear hydrogen bonds (O···O 2.460(2) A). The piperazine ring adopts a chair conformation with the CH2COOH group in the axial and the Me group in the equatorial positions. The N+ atoms interact electrostatically with the Cl- ion and the oxygen atoms of the carboxylate groups. The FTIR spectrum of 7-Cl shows an intense broad absorption in the 1500-400 cm-1 region and a νC:O band at 1734 cm-1. The pKa values of I and II were determined by potentiometric titration The 1H and 13C NMR spectra in D2O were analyzed.

CC 22-12 (Physical Organic Chemistry)
Section cross-reference(s): 75

IT 488721-89-7P 488721-90-0P **488721-93-3P 488721-94-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, mol. structure, hydrogen bonding, basicity and spectroscopic properties of N,N'-dimethylpiperazine betaines and their hydrohalides)

IT **488721-93-3P 488721-94-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, mol. structure, hydrogen bonding, basicity and spectroscopic properties of N,N'-dimethylpiperazine betaines and their hydrohalides)

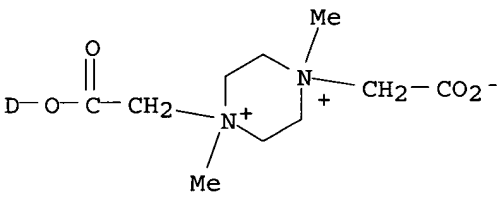
RN 488721-93-3 CAPLUS
CN Piperazinium, 1-(carboxy-d-methyl)-1,4-dimethyl-, chloride, hydrochloride-d (9CI) (CA INDEX NAME)



● Cl⁻

● DCl

RN 488721-94-4 CAPLUS
CN Piperazinium, 1,4-bis(carboxy-d-methyl)-1,4-dimethyl-, inner salt, chloride (9CI) (CA INDEX NAME)



● Cl⁻

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:748069 CAPLUS
DOCUMENT NUMBER: 130:106840
TITLE: A Light-Activated Antibody Catalyst
AUTHOR(S): Taylor, Matthew J.; Hoffman, Timothy Z.; Yli-Kauhaluoma, Jari T.; Lerner, Richard A.; Janda, Kim D.
CORPORATE SOURCE: Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of the American Chemical Society (1998), 120(49), 12783-12790
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:106840
AB A catalytic antibody for a multistep Norrish type II photochem. reaction was investigated. Absorption of light energy by an α-ketoamide substrate produced a high-energy biradical intermediate, that was then directed by the antibody microenvironment to form tetrahydropyrazine with a kcat of 1.4 + 10-3 min-1 at 280 nm irradiation and an enantiomeric

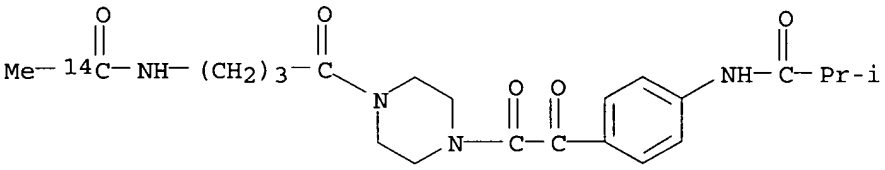
excess of 78%. Antibody-catalyzed reactions performed with radiolabeled substrate indicated that little self-inactivation (6.8 mol % covalent modification after four turnovers per antibody) occurred. The singular product obtained in the antibody-catalyzed reaction was not observed in the uncatalyzed reaction unless the pH was lowered below 4. Studies suggested that the interplay of conformational control and chemical catalysis were responsible for the high specificity. A change in protonation state of the antibody was correlated with the inclusion of a new reaction pathway in the antibody-catalyzed reaction, indicating that general-base catalysis was involved in the rerouting of the Norrish reaction to form tetrahydropyrazine. An x-ray crystal structure of the substrate was obtained and suggested that the antibody binds the α-ketoamide in a twisted conformation optimal for the first step of the photochem. reaction. The antibody described here is a model for the evolution of light-activated enzymes and can serve as a foundation for the development of light-dependent antibody catalysts for a range of even more complex photochem. reactions.

CC 7-4 (Enzymes)
Section cross-reference(s): 75

IT 219661-57-1P 219661-59-3P **219661-64-0P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(synthesis of substrates for a light-activated antibody catalyst of a Norrish type II photochem. reaction)

IT **219661-64-0P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(synthesis of substrates for a light-activated antibody catalyst of a Norrish type II photochem. reaction)

RN 219661-64-0 CAPLUS
CN Propanamide, N-[4-[[4-[4-(acetyl-1-14C-amino)-1-oxobutyl]-1-piperazinyl]oxoacetyl]phenyl]-2-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:430484 CAPLUS
DOCUMENT NUMBER: 125:131552
TITLE: Replacing 14C with stable isotopes in drug metabolism studies
AUTHOR(S): Abramson, Fred P.; Teffera, Yohannes; Kusmierz, Josef; Steenwyk, Rick C.; Pearson, Paul G.
CORPORATE SOURCE: Dep. Pharmacol., George Washington Univ. Sch. Med. Health Sci., Washington, DC, 20037, USA
SOURCE: Drug Metabolism and Disposition (1996), 24(7), 697-701
CODEN: DMDSAI; ISSN: 0090-9556
PUBLISHER: Williams & Wilkins

DOCUMENT TYPE: Journal
LANGUAGE: English

AB After administration of a mixed dose of both radioisotope and stable-isotope-labeled tirilazad, the authors carried out a parallel set of HPLC analyses for drug metabolites in bile samples from monkeys and dogs using either radioactivity monitoring (RAM) for 14C or the chemical reaction interface mass spectrometry technique (CRIMS) to detect 13C or 15N. CRIMS is a novel method where analytes are decomposed in a microwave-induced plasma and the elements contained in the analytes are reformulated into small gaseous species that are detected by a mass spectrometer. The comprehensiveness of detection, chromatog. resolution, sensitivity, signal/noise, and quant. abilities of CRIMS were compared with RAM and in no case was RAM superior. This implies that stable isotopes may be substituted for radioisotopes in studies of drug metabolism where the ability of the latter approach to detect a label independent of the structures in which the label appears has been the primary reason for continuing to use a hazardous and expansive tracer. With HPLC-CRIMS, stable isotopes such as 13C and 15N can be comprehensively detected and quant. patterns of drug metabolism from biol. fluids can be produced that mirror the results when 14C is used.

CC 1-2 (Pharmacology)

IT 110101-67-2, Tirilazad mesylate **161860-83-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(replacing 14C with stable isotopes in drug metabolism studies using chemical
reaction interface mass spectrometry in relation to tirilazad metabolism)

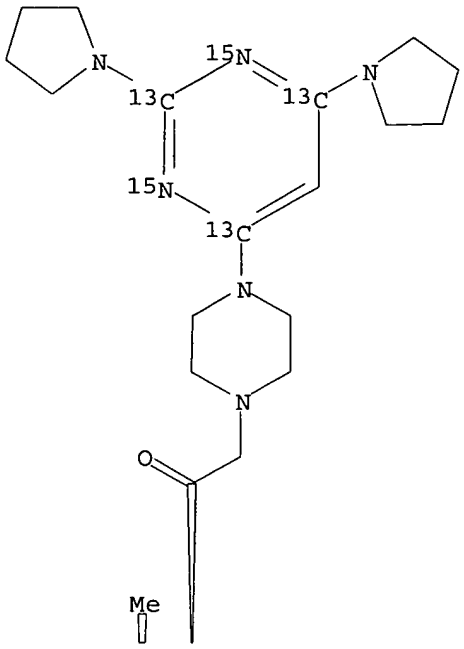
IT **161860-83-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(replacing 14C with stable isotopes in drug metabolism studies using chemical
reaction interface mass spectrometry in relation to tirilazad metabolism)

RN 161860-83-9 CAPLUS

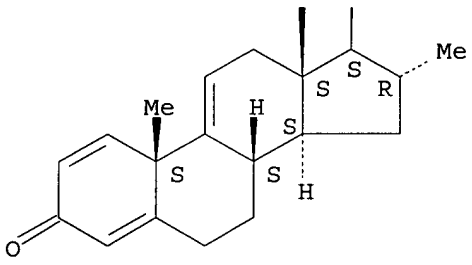
CN Pregna-1,4,9(11)-triene-3,20-dione, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl-2,4,6-13C3-1,3-15N2)-1-piperazinyl]-16-methyl-, (16α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



L30 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:262564 CAPLUS
DOCUMENT NUMBER: 122:214319
TITLE: Synthesis of radioactive and stable isotope labeled tirilazad mesylate
AUTHOR(S): Stolle, W. T.; Easter, J. A.; Chew, E. H.; McGarth, J. P.; Palmer, J. R.; Hsi, R. S. P.
CORPORATE SOURCE: Upjohn Laboratories, The Upjohn Co., Kalamazoo, MI, 49001, USA
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1994), 34(12), 1187-99
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Several isotopically labeled versions of tirilazad mesylate,

21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-16α-methylpregna-1,4,9(11)-triene-3,20-dione monomethanesulfonate, have been synthesized for conducting in vitro and in vivo metabolic transformations of this exptl. drug. These include labeling with carbon-14 at the 16α-Me group of the steroid portion of the mol., or at the C-2 position of the pyrimidine ring; also with deuterium at the steroid 16α-Me group, and/or with carbon-13 at C-2, C-4, and C-6, and with nitrogen-15 at N-1 and N-3 of the pyrimidine ring.

CC 32-5 (Steroids)

IT 110101-67-2DP, Tirilazad mesylate, labeled derivs. **161860-82-8P 161860-84-0P 161860-86-2P 161860-88-4P 161860-90-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of radioactive and stable isotope labeled tirilazad mesylate)

IT **161860-82-8P 161860-84-0P 161860-86-2P 161860-88-4P 161860-90-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of radioactive and stable isotope labeled tirilazad mesylate)

RN 161860-82-8 CAPLUS

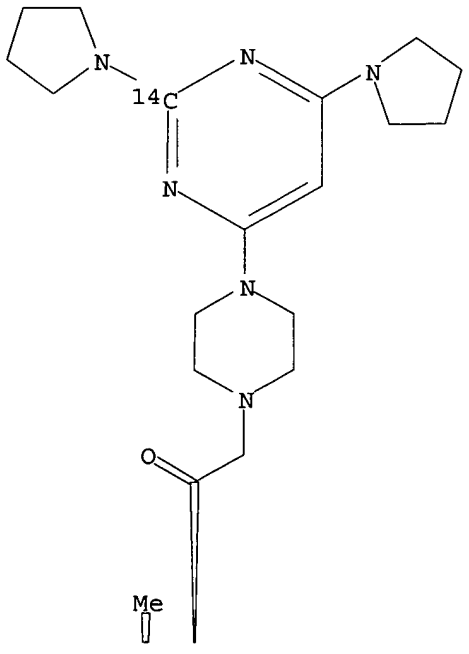
CN Pregna-1,4,9(11)-triene-3,20-dione, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl-2-14C)-1-piperazinyl]-16-methyl-, (16α)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

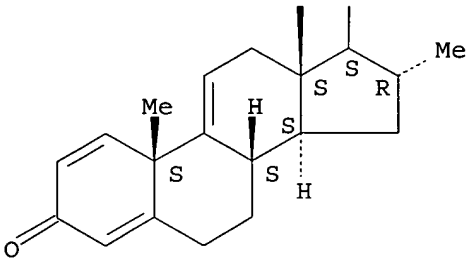
CRN 161860-81-7
CMF C38 H52 N6 O2

Absolute stereochemistry.

PAGE 1-A

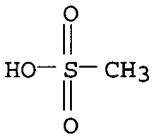


PAGE 2-A



CM 2

CRN 75-75-2
CMF C H4 O3 S



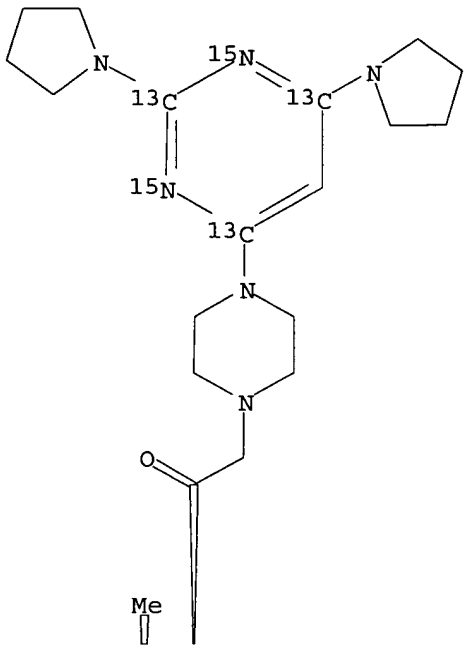
RN 161860-84-0 CAPLUS
CN Pregna-1,4,9(11)-triene-3,20-dione, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl-2,4,6-13C3-1,3-15N2)-1-piperazinyl]-16-methyl-, monomethanesulfonate, (16α)- (9CI) (CA INDEX NAME)

CM 1

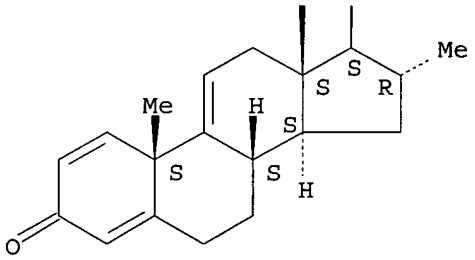
CRN 161860-83-9
CMF C38 H52 N6 O2

Absolute stereochemistry.

PAGE 1-A

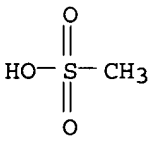


PAGE 2-A



CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 161860-86-2 CAPLUS
CN Pregna-1,4,9(11)-triene-3,20-dione, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-16-(methyl-d3)-, monomethanesulfonate,

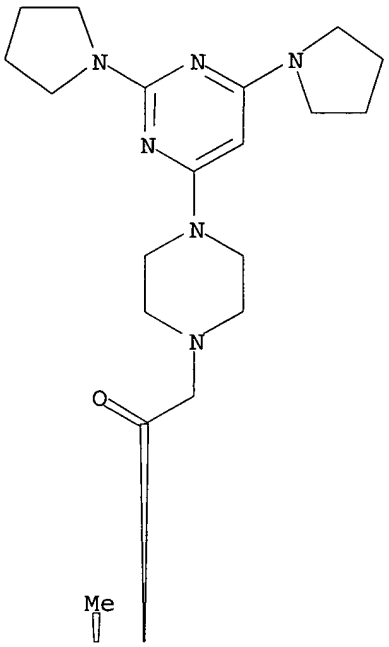
(16α)- (9CI) (CA INDEX NAME)

CM 1

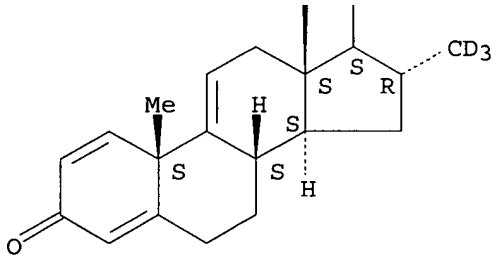
CRN 161860-85-1
CMF C38 H49 D3 N6 O2

Absolute stereochemistry.

PAGE 1-A

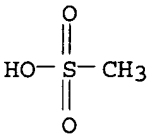


PAGE 2-A



CM 2

CRN 75-75-2
CMF C H4 O3 S



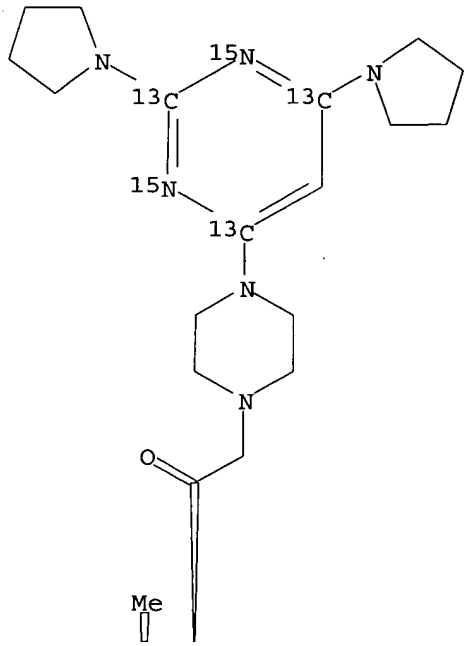
RN 161860-88-4 CAPLUS
CN Pregna-1,4,9(11)-triene-3,20-dione, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl-2,4,6-13C3-1,3-15N2)-1-piperazinyl]-16-(methyl-d3)-, monomethanesulfonate, (16α)- (9CI) (CA INDEX NAME)

CM 1

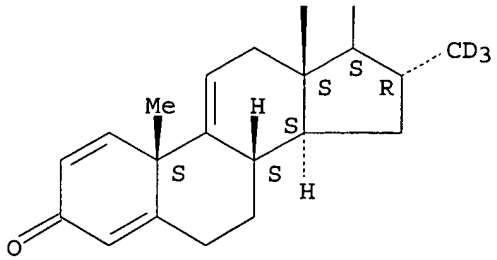
CRN 161860-87-3
CMF C38 H49 D3 N6 O2

Absolute stereochemistry.

PAGE 1-A

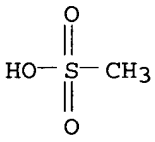


PAGE 2-A



CM 2

CRN 75-75-2
CMF C H4 O3 S

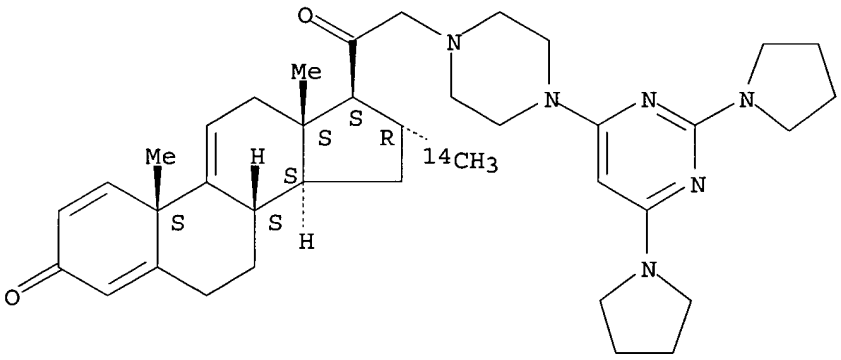


RN 161860-90-8 CAPLUS
CN Pregna-1,4,9(11)-triene-3,20-dione, 21-[4-(2,6-di-1-pyrrolidinyl-4-pyrimidinyl)-1-piperazinyl]-16-(methyl-14C)-, monomethanesulfonate, (16α)- (9CI) (CA INDEX NAME)

CM 1

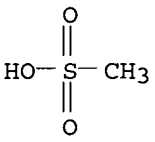
CRN 161860-89-5
CMF C38 H52 N6 O2

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S

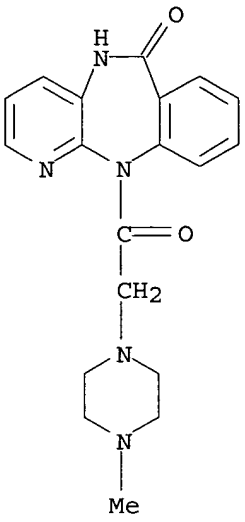


L30 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:102104 CAPLUS
DOCUMENT NUMBER: 116:102104

TITLE: Recent trends in receptor analysis techniques and instrumentation
AUTHOR(S): Palacios, J. M.; Mengod, G.; Vilaro, M. T.; Ramm, P.
CORPORATE SOURCE: Sandoz Pharma Ltd., Basel, 4002, Switz.
SOURCE: Journal of Chemical Neuroanatomy (1991), 4(5), 343-53
CODEN: JCNAEE; ISSN: 0891-0618
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Receptor autoradiog. allows visualization of receptor binding sites at the regional or light microscopic level. Receptor autoradiog. is a mature methodol., in widespread use. It is also a dynamic and expanding methodol., benefiting constantly from the introduction of new techniques and instrumentation. In particular, receptor autoradiog. has taken advantage of image anal. instrumentation to provide efficient spatial mapping of receptor populations and their pharmacol. characteristics. A major contribution to the understanding of receptors has come from the recent cloning of the genes coding for many of these receptors. This has allowed the use of in situ hybridization to demonstrate the cells expressing mRNA coding for specific receptor subtypes. The result is that many receptor populations, previously thought to be homogeneous, are shown to be composed of several subtypes. As a consequence, the distribution of many receptors requires re-examination, which is aided by the development of new and more selective ligands. With the incorporation of techniques from mol. biol. into receptor autoradiog., the demands upon image anal. instruments have expanded. Over the past decade, densitometric image anal. have attained a high level of sophistication for classical receptor autoradiog. However, to serve the needs of today's receptor laboratory, an image analyzer must be equally capable in regional densitometry, in counting and spatial mapping of grain and or cell locations at the microscopic level, and in analyzing electrophoresis gels. Advances in image anal. hardware and software are keeping pace with the requirements of receptor labs. As an example, the authors illustrated here some of their results with muscarinic receptors.

CC 9-8 (Biochemical Methods)
IT 83945-36-2 **124620-97-9** 131042-02-9 139182-85-7 140186-38-5
RL: ANST (Analytical study)
(autoradiog. with, of muscarinic receptors in brain, image anal. requirements for)
IT **124620-97-9**
RL: ANST (Analytical study)
(autoradiog. with, of muscarinic receptors in brain, image anal. requirements for)
RN 124620-97-9 CAPLUS
CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)

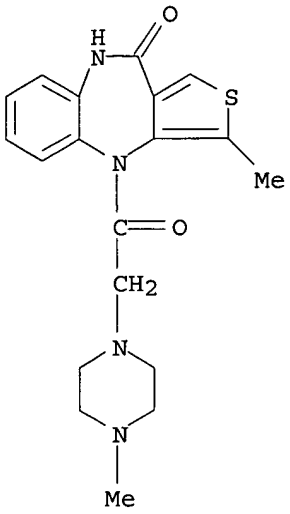


L30 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:452079 CAPLUS
DOCUMENT NUMBER: 113:52079
TITLE: Telenzepine enantiomers block muscarinic M1-receptors with opposite kinetics
AUTHOR(S): Eltze, Manfrid
CORPORATE SOURCE: Dep. Pharmacol., Byk Gulden Pharm., Konstanz, D-7750, Germany
SOURCE: European Journal of Pharmacology (1990), 180(1), 161-8
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English

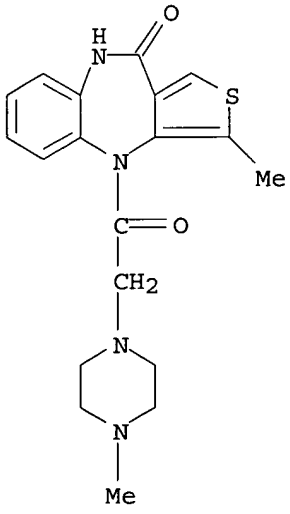
AB Stimulation of muscarinic M1-receptors in isolated rabbit vas deferens by McN-A-343 inhibited elec. induced twitch contractions, an effect which was competitively antagonized by (+)-, (±)-, and (-)-telenzepine and pirenzepine (pA2 = 9.12, 8.86, 6.98, and 7.79, resp.). The inhibition of twitch contractions by 10-6M McN-A-343 was reversed by the antimuscarinic agents (at concns. 10-fold higher than pA2) in a time-dependent manner. The antagonists were then displaced by 3 + 10-5M McN-A-343, which again led to inhibition of twitch contractions. Assuming 1st-order kinetics for M1-receptor blockade by the antagonists, half-time values for the start and end of blockade were calculated For (+)-telenzepine, the values for the rates for the start and end of blockade were 23 and 174 min, resp., whereas (-)-telenzepine exhibited an inverse kinetic pattern of 3.0 and 0.38 min, resp. The extremely slow dissociation of (+)-telenzepine from muscarinic M1-receptors may explain the long-lasting pharmacol. effect of this compound in vivo.

CC 1-3 (Pharmacology)
IT 28797-61-7, Pirenzepine **122195-38-4 122195-39-5 122219-70-9**
RL: BIOL (Biological study)
(muscarinic M1 receptors blockade by, kinetics of, stereoisomerism in relation to)
IT **122195-38-4 122195-39-5 122219-70-9**
RL: BIOL (Biological study)
(muscarinic M1 receptors blockade by, kinetics of, stereoisomerism in relation to)
RN 122195-38-4 CAPLUS

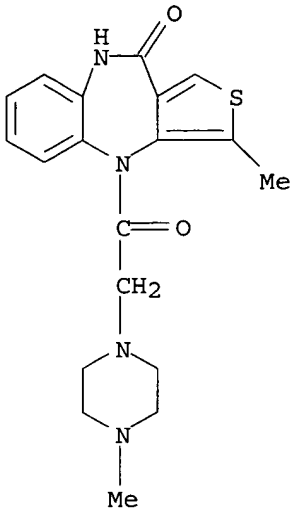
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (+)- (9CI) (CA INDEX NAME)



RN 122195-39-5 CAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (-)- (9CI) (CA INDEX NAME)



RN 122219-70-9 CAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



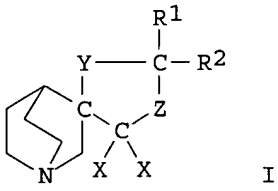
L30 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:48812 CAPLUS
DOCUMENT NUMBER: 112:48812
TITLE: Novel oxathiolane derivatives their preparation, and their therapeutic use
INVENTOR(S): Fisher, Abraham; Karton, Ishai
PATENT ASSIGNEE(S): Israel Institute for Biological Research, Israel
SOURCE: Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 314444	A2	19890503	EP 1988-310040	19881026
EP 314444	A3	19901107		
EP 314444	B1	19960529		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE				
US 4876260	A	19891024	US 1988-189210	19880502
IL 87834	A1	19920525	IL 1988-87834	19880922
ZA 8807326	A	19891129	ZA 1988-7326	19880929
AU 8823671	A1	19890504	AU 1988-23671	19881012
AU 608903	B2	19910418		
AT 138663	E	19960615	AT 1988-310040	19881026
ES 2087854	T3	19960801	ES 1988-310040	19881026
DK 8805986	A	19890429	DK 1988-5986	19881027
DK 175064	B1	20040517		
NO 8804790	A	19890502	NO 1988-4790	19881027
NO 167806	B	19910902		
NO 167806	C	19911211		
CA 1315791	A1	19930406	CA 1988-581526	19881027
JP 02062883	A2	19900302	JP 1988-271085	19881028
JP 2753280	B2	19980518		
IN 170689	A	19920502	IN 1990-MA426	19900530
IN 170320	A	19920314	IN 1990-MA455	19900611
PRIORITY APPLN. INFO.:			US 1987-114473 A	19871028

US 1988-189210 A 19880502
IN 1988-MA695 A 19881005

OTHER SOURCE(S): CASREACT 112:48812; MARPAT 112:48812

GI



I

AB Spiro-oxathiolane/quinuclidine derivs. I [1 of Y and Z = O and the other is S(O)n (n = 0-2); R1, R2 = H, alkyl, alkenyl, etc. (at least R1 or R2 ≠ H); X = H (or when Y = O and Z = S(O)n simultaneously, X = 2H, 3H), etc.] and their geometric isomers, enantiomers, diastereomers, racemates, and acid addition salts, and pharmaceutical compns. containing them, are provided. I are useful as medicaments or diagnostic agents, or in the manufacture of medicaments and diagnostic agents, applicable to diseases or disorders of the central nervous or cholinergic system. Ten derivs. were tested for their ability, as compared with oxotremorine (mainly an M2 muscarinic receptor agonist) and McN-A-343 (mainly an M1 muscarinic receptor agonist), to displace tritiated quinuclidinyl benzilate (3H-QNB) from rat brain homogenates. The (-)-cis-2-methylspiro(1,3-oxathiolan-5,3')quinulcidine was 2.2 times more potent in 3H-QNB displacement than its racemate. Moreover, the latter was the most selective M1 agonist, being more selective than the prototype M1 agonist McN-A-343.

IC ICM C07D497-20
ICS C07B059-00; A61K031-435; A61K043-00

ICI C07D497-20, C07D327-00, C07D221-00

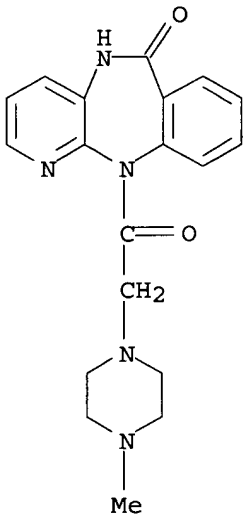
CC 1-11 (Pharmacology)
Section cross-reference(s): 28

IT 70761-70-5 **124620-97-9** 124620-98-0
RL: BIOL (Biological study)
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)

IT **124620-97-9**
RL: BIOL (Biological study)
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)

RN 124620-97-9 CAPLUS

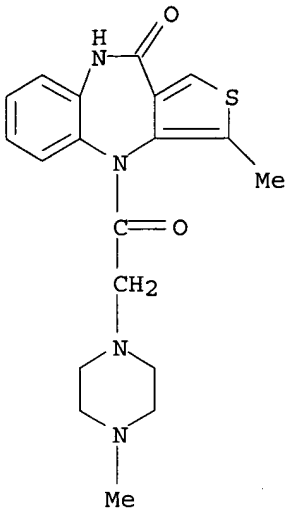
CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



L30 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:151426 CAPLUS
DOCUMENT NUMBER: 112:151426
TITLE: Cyproheptadine displays high affinity for muscarinic receptors but does not discriminate between receptor subtypes
AUTHOR(S): Eltze, Manfrid; Lambrecht, Guenter; Mutschler, Ernst
CORPORATE SOURCE: Dep. Pharmacol., Byk Gulden Pharm., Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: European Journal of Pharmacology (1989), 173(2-3), 219-22
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The affinity of cyproheptadine for different muscarinic receptor subtypes was investigated in vitro by functional expts. in field-stimulated vas deferens of the rabbit (ganglionic M1- and cardiac M2-receptors) and in guinea pig ileum (smooth muscle M3-receptors). Cyproheptadine displayed high but similar affinity for all muscarinic receptor subtypes studied (pA2 = 7.99-8.02). In contrast, (+)-telenzepine (M1 over M2 and M3) and mefurtramine (M2 over M3 and M1) were selective.

CC 1-7 (Pharmacology)
IT **122195-38-4** 126116-01-6
RL: BIOL (Biological study)
(muscarinic receptor subtypes response to, specificity of, cyproheptadine in relation to)
IT **122195-38-4**
RL: BIOL (Biological study)
(muscarinic receptor subtypes response to, specificity of, cyproheptadine in relation to)
RN 122195-38-4 CAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (+)- (9CI) (CA INDEX NAME)

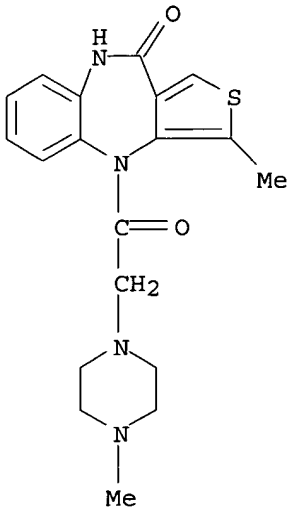


L30 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:490172 CAPLUS
DOCUMENT NUMBER: 111:90172
TITLE: The affinity, selectivity and biological activity of telenzepine enantiomers
AUTHOR(S): Schudt, C.; Boer, R.; Eltze, M.; Riedel, R.; Grundler, G.; Birdsall, N. J. M.
CORPORATE SOURCE: Dep. Pharmacol., Byk Gulden Res. Lab., Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: European Journal of Pharmacology (1989), 165(1), 87-96
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English

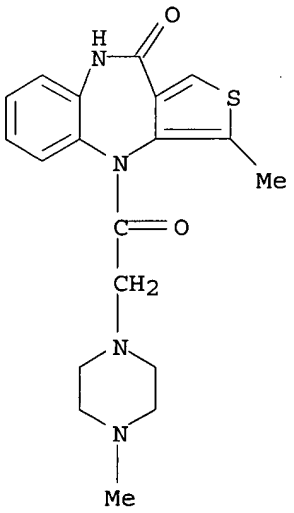
AB The binding of the enantiomers of telenzepine, an antiulcer drug, to muscarinic receptor subtypes in the guinea-pig cerebral cortex, myocardium and salivary glands was examined The (+)-enantiomer was more potent in all assays and exhibited a greater selectivity than the (-)-enantiomer for the different receptor subtypes in membrane prepns.. The enantiomeric potency ratio varied from .simeq.400 (cortical M1 receptors) to .simeq.50 (cardiac receptors). In functional assays in vitro in the rabbit vas deferens and rat atria, the affinity consts. and enantiomeric potency ratios for the 2 isomers agreed with those found in the binding assays. A high enantiomeric potency ratio, 180, was found in vivo for the ability of the telenzepine enantiomers to inhibit the production of stomach mucosal lesions in the modified Shay rat preparation The data are compatible with the blockade of M1 receptors by (+)-telenzepine and oppose the possibility that the anti-ulcer action of telenzepine is mediated via a muscarinic or non-muscarinic action of the (-)-enantiomer.

CC 1-9 (Pharmacology)
IT **122195-38-4 122195-39-5 122219-70-9**
RL: BIOL (Biological study)
(muscarinic receptor-blocking activity of, in ulcer inhibition, stereochem. in)
IT **122195-38-4 122195-39-5 122219-70-9**
RL: BIOL (Biological study)
(muscarinic receptor-blocking activity of, in ulcer inhibition, stereochem. in)
RN 122195-38-4 CAPLUS

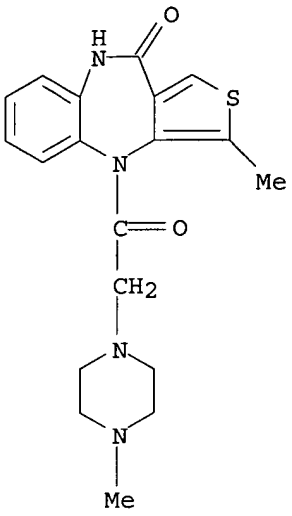
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (+)- (9CI) (CA INDEX NAME)



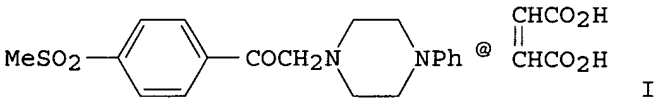
RN 122195-39-5 CAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium, (-)- (9CI) (CA INDEX NAME)



RN 122219-70-9 CAPLUS
CN 10H-Thieno[3,4-b][1,5]benzodiazepin-10-one, 4,9-dihydro-3-methyl-4-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



L30 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:114197 CAPLUS
DOCUMENT NUMBER: 94:114197
TITLE: Biochemistry of drugs. XXVI. Pharmacokinetics of 1-(4-methanesulfonylphenacyl)-4-phenylpiperazine maleinate (mesylphenacyrazine) in rats
AUTHOR(S): Franc, Z.; Smolik, S.; Horesovsky, O.
CORPORATE SOURCE: Vyzk. Ustav Farm. Biochem., Prague, Czech.
SOURCE: Cesko-Slovenska Farmacie (1980), 29(8-9), 290-3
CODEN: CKFRAY; ISSN: 0009-0530
DOCUMENT TYPE: Journal
LANGUAGE: Czech
GI



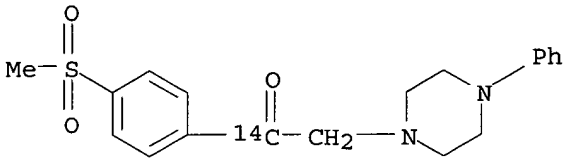
I

AB 14C-labeled 1-(4-methanesulfonylphenacyl)-4-phenylpiperazine maleinate (I) [50648-51-6] (15 mg/kg, orally) was rapidly absorbed and excreted in rats. Half of the radioactivity was excreted in 15 h. The dose of 150 mg I/kg was absorbed and excreted at a substantially slower rate than higher doses. Half the administered radioactivity was excreted in urine and feces in 24 h or longer. The tissue distribution of I and its metabolites from high to low affinity was in the order: liver, kidneys, lungs, spleen, brain, testis, heart, skin, muscle, and eye. N-Phenylpiperazine [92-54-6], maleic acid [110-16-7], 1-(4-methanesulfonylphenacyl)-4-(p-hydroxyphenyl)piperazine [56621-49-9], and 1-(methanesulfonylphenyl)-2-(4-phenylpiperazinyl)ethanol [56621-54-6] were identified as I metabolites in urine. No I was found in urine.
CC 1-2 (Pharmacodynamics)
IT **76713-14-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **76713-14-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 76713-14-9 CAPLUS
CN Ethanone-1-14C, 1-[4-(methylsulfonyl)phenyl]-2-(4-phenyl-1-piperazinyl)-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

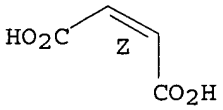
CRN 76713-13-8
CMF C19 H22 N2 O3 S



CM 2

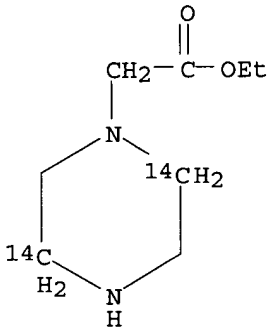
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



L30 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:475189 CAPLUS
DOCUMENT NUMBER: 77:75189
TITLE: Synthesis of ethyl 4-(3,4,5-trimethoxycinamoyl)-[2,5-14C]piperazinyl acetate and ethyl 4-(3,4,5-trimethoxy[β-14C]cinnamoyl)piperazinyl acetate
AUTHOR(S): Hardy, G.; Sword, I. P.; Hathway, D. E.
CORPORATE SOURCE: Dep. Metab. Stud., Huntingdon Res. Cent., Huntingdon, UK
SOURCE: Journal of Labelled Compounds (1972), 8(2), 221-30
CODEN: JLCAAI; ISSN: 0022-2135
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Et 4-(3,4,5-trimethoxycinnamoyl)piperazinyl-2,5-14C acetate was prepared from piperazine-2,5-14C, and Et piperazinyl-2,5-14C acetate, and Et 4-(3,4,5-trimethoxycinnamoyl-β-14C)-piperazinyl acetate was prepared from 3,4,5-trimethoxybromobenzene and 3,4,5-trimethoxybenzaldehyde-α-14C.
CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 2539-27-7P 2675-79-8P 37024-12-7P **37024-13-8P**
37024-14-9P 37024-16-1P **38420-54-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

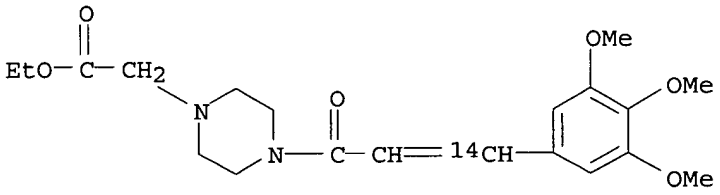
IT **37024-13-8P 37024-14-9P 38420-54-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 37024-13-8 CAPLUS
CN 1-Piperazine-2,5-14C2-acetic acid, ethyl ester (9CI) (CA INDEX NAME)



RN 37024-14-9 CAPLUS
CN 1-Piperazineacetic acid, 4-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-propenyl-3-14C]-, ethyl ester, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

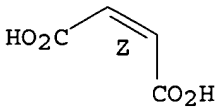
CRN 47588-13-6
CMF C20 H28 N2 O6



CM 2

CRN 110-16-7
CMF C4 H4 O4

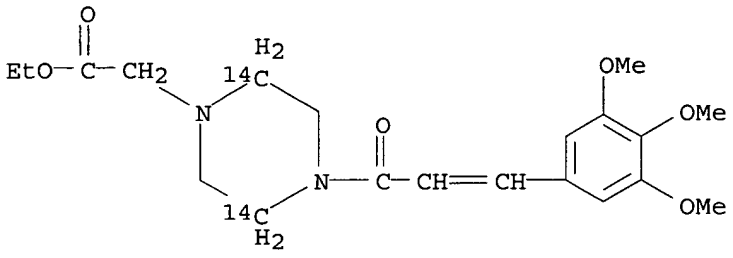
Double bond geometry as shown.



RN 38420-54-1 CAPLUS
CN 1-Piperazine-2,5-14C2-acetic acid, 4-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-propenyl]-, ethyl ester, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

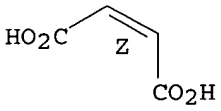
CRN 47588-14-7
CMF C20 H28 N2 O6



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



L30 ANSWER 22 OF 25 USPATFULL on STN
ACCESSION NUMBER: 2005:57488 USPATFULL
TITLE: Isotopically coded affinity markers 3
INVENTOR(S): Lerchen, Hans-Georg, Leverkusen, GERMANY, FEDERAL REPUBLIC OF
Siegmund, Hans-Ulrich, Leverkusen, GERMANY, FEDERAL REPUBLIC OF
Immler, Dorian, Leverkusen, GERMANY, FEDERAL REPUBLIC OF
Schumacher, Andreas, Erfringen, GERMANY, FEDERAL REPUBLIC OF
Auriel, Daniel, Fallingbostel, GERMANY, FEDERAL REPUBLIC OF

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2005049406	A1	20050303	
APPLICATION INFO.:	US 2004-494999	A1	20041029	(10)
	WO 2002-EP12105		20021030	

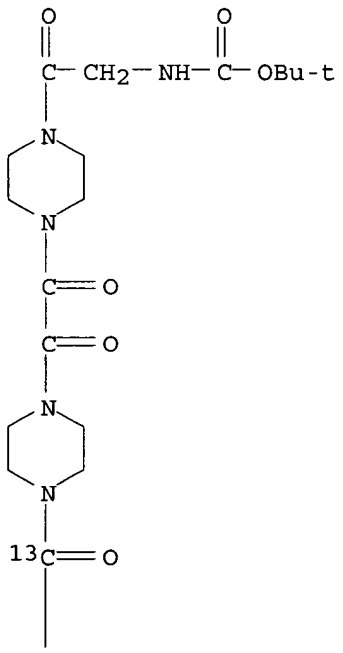
	NUMBER	DATE
PRIORITY INFORMATION:	DE 2001-154	20011109
	DE 2002-102	20020729

DOCUMENT TYPE: Utility

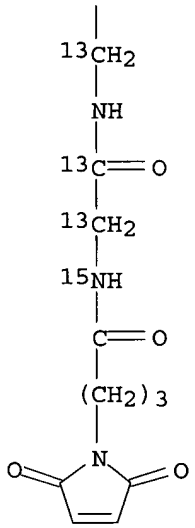
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: JEFFREY M. GREENMAN, BAYER PHARMACEUTICALS CORPORATION, 400 MORGAN LANE, WEST HAVEN, CT, 06516
NUMBER OF CLAIMS: 16
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 4 Drawing Page(s)
LINE COUNT: 2051
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention concerns isotopically coded affinity markers (ICAT) for mass spectrometric analysis of proteins, and the preparation and use if said markers.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **525587-68-2P 525587-70-6P 525587-72-8P**
(preparation and N-deprotection of; preparation of isotopically-coded affinity
markers for mass spectrometric anal. of proteins)
RN 525587-68-2 USPATFULL
CN Carbamic acid, [2-[4-[[4-[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]oxoacetyl]-1-piperazinyl]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

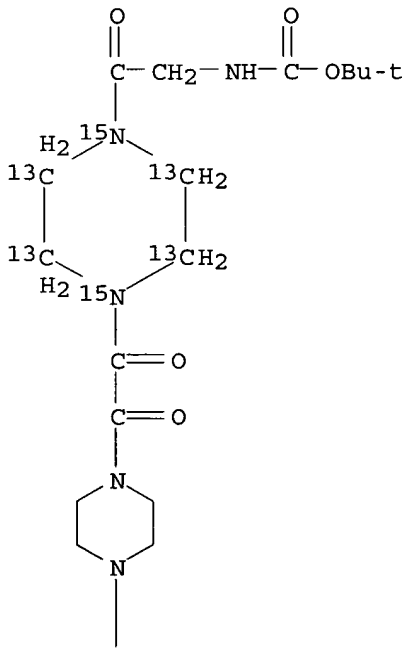


PAGE 2-A



RN 525587-70-6 USPATFULL
CN Carbamic acid, [2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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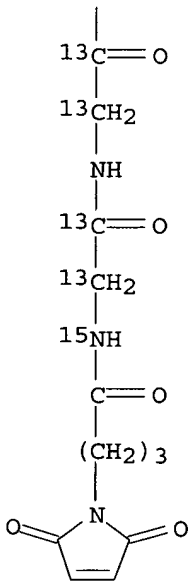
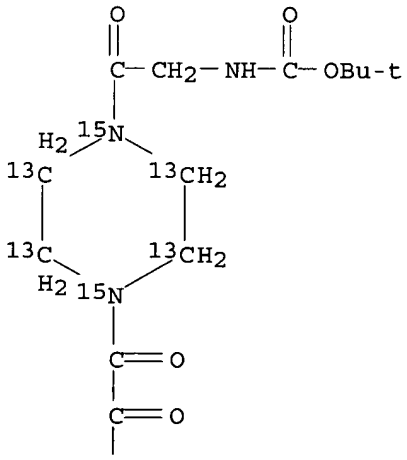
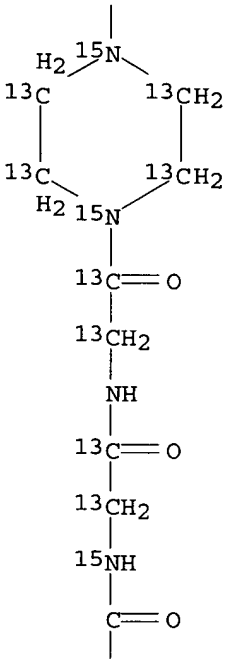


RN 525587-72-8 USPATFULL
CN Carbamic acid, [2-[4-[[4-[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

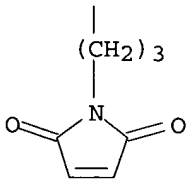
PAGE 1-A



PAGE 2-A

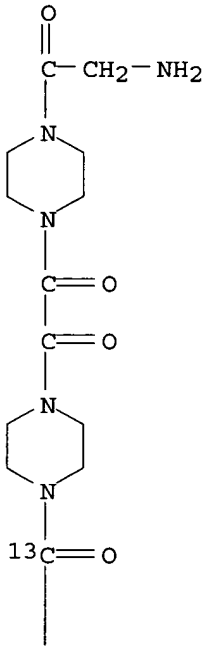


PAGE 3-A

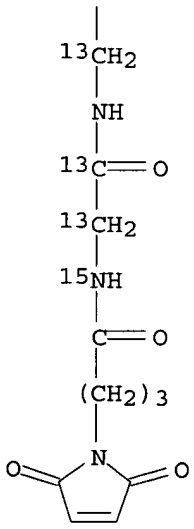


IT **525587-69-3P 525587-71-7P 525587-73-9P**
(preparation and coupling of, with biotin derivative; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)
RN 525587-69-3 USPATFULL
CN 1H-Pyrrole-1-butanamide-15N, N-[2-[[2-[4-[[4-(aminoacetyl)-1-piperazinyl]oxoacetyl]-1-piperazinyl]-2-oxoethyl-13C2]amino]-2-oxoethyl-13C2]-2,5-dihydro-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 1-A

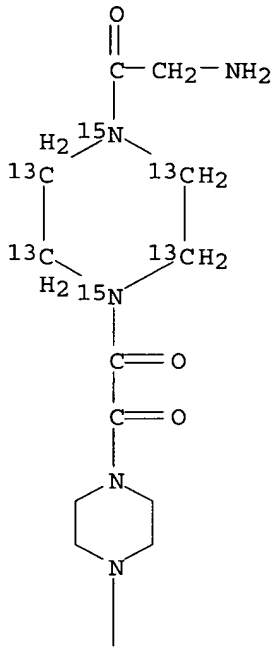


PAGE 2-A

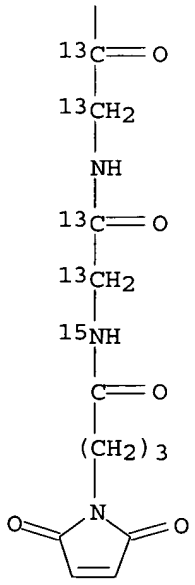


RN 525587-71-7 USPATFULL
CN 1H-Pyrrole-1-butanamide-15N, N-[2-[[2-[4-[[4-(aminoacetyl)-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]oxoacetyl]-1-piperazinyl]-2-oxoethyl-13C2]amino]-2-oxoethyl-13C2]-2,5-dihydro-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 1-A

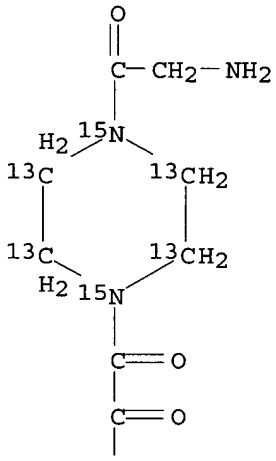


PAGE 2-A



RN 525587-73-9 USPATFULL
CN 1H-Pyrrole-1-butanamide-15N, N-[2-[[2-[4-[[4-(aminoacetyl)-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl-13C2]amino]-2-oxoethyl-13C2]-2,5-dihydro-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 1-A



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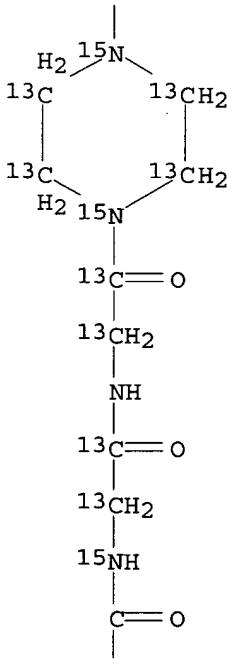
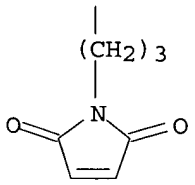


PAGE 3-A



IT **525587-28-4P 525587-30-8P 525587-32-0P**
(preparation and reaction of, with biotin derivative; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)
RN 525587-28-4 USPATFULL
CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinylacetyl)-1-piperazinyl]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 525587-27-3
CMF C22 H31 N7 O7

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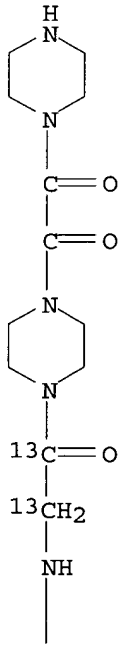

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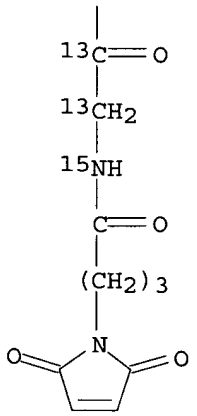
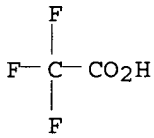


CM 2

CRN 76-05-1
CMF C2 H F3 O2

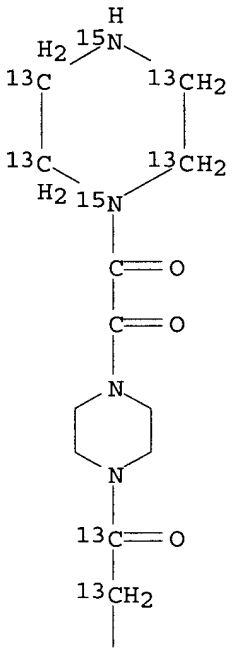


RN 525587-30-8 USPATFULL
CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-acetyl)-1-piperazinyl]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 525587-29-5
CMF C22 H31 N7 O7

PAGE 1-A



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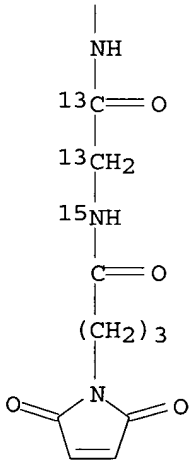
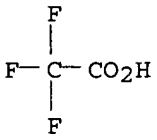


CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 525587-32-0 USPATFULL
CN 1H-Pyrrole-1-butanamide-15N, 2,5-dihydro-2,5-dioxo-N-[2-oxo-2-[[2-oxo-2-[4-(oxo-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-acetyl)-1-piperazinyl-2,3,5,6-13C4-1,4-15N2-]ethyl-13C2]amino]ethyl-13C2]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 525587-31-9
CMF C22 H31 N7 O7

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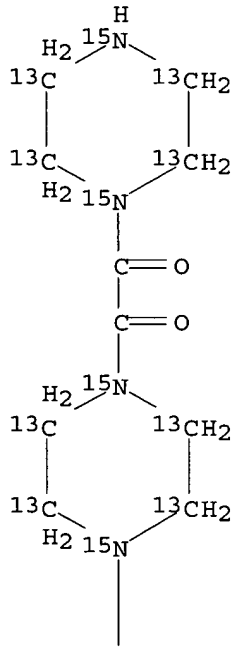

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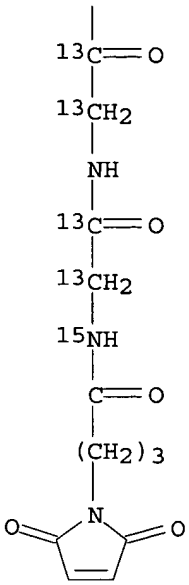
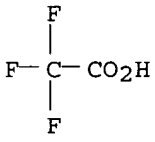


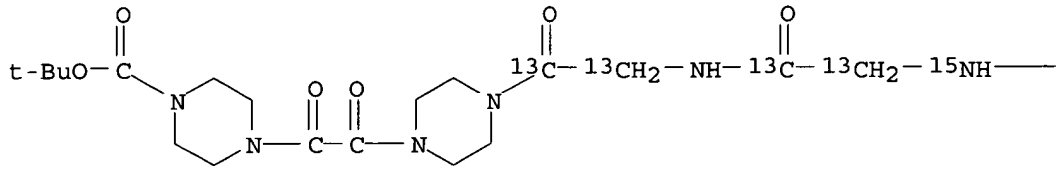
CM 2

CRN 76-05-1
CMF C2 H F3 O2



IT **525587-24-0P 525587-25-1P 525587-26-2P**
(preparation and regioselective N-deprotection of; preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)
RN 525587-24-0 USPATFULL
CN 1-Piperazinecarboxylic acid, 4-[oxo[4-[[[[[(phenylmethoxy)carbonyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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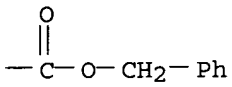

RN 525587-25-1 USPATFULL
CN 1-Piperazine-2,3,5,6-13C4-1,4-15N2-carboxylic acid, 4-[oxo[4-[[[[[(phenylmethoxy)carbonyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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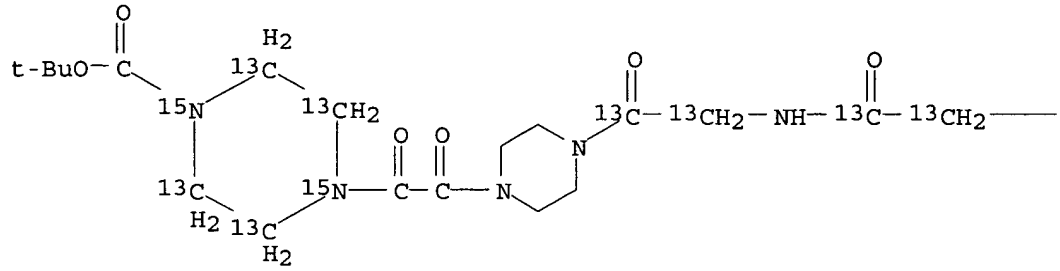

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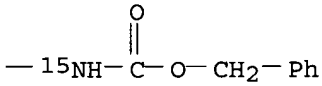

RN 525587-26-2 USPATFULL
CN 1-Piperazine-2,3,5,6-13C4-1,4-15N2-carboxylic acid, 4-[oxo[4-[[[[[(phenylmethoxy)carbonyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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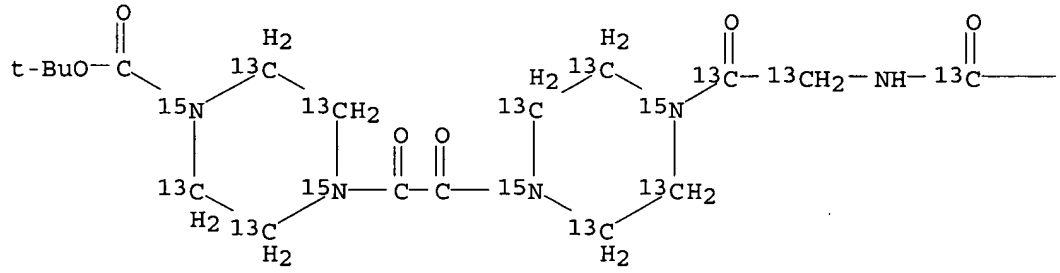

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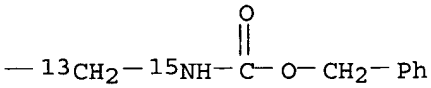


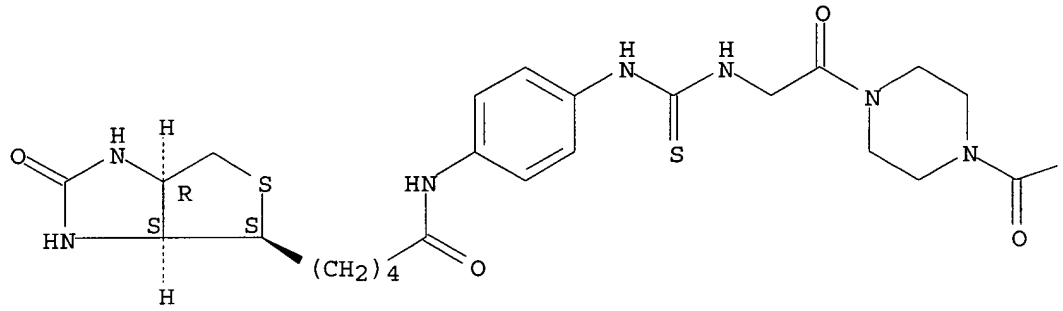
IT **525586-79-2P 525586-80-5P 525586-81-6P**
(preparation of isotopically-coded affinity markers for mass spectrometric anal. of proteins)

RN 525586-79-2 USPATFULL

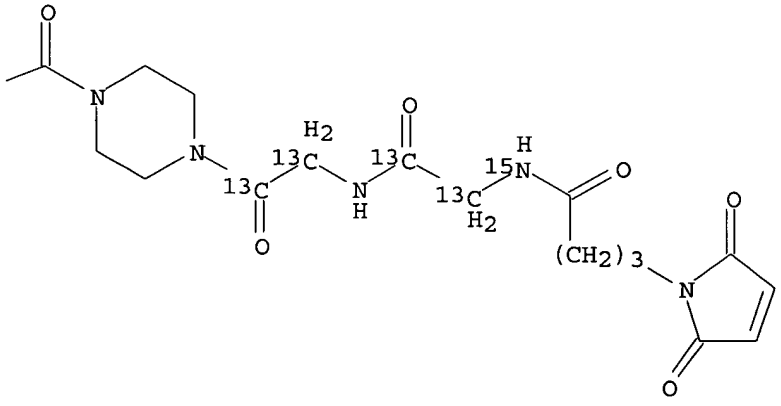
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[4-[[[[2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]oxoacetyl]-1-piperazinyl]-2-oxoethyl]amino]thioxomethyl]amino]phenyl]hexahydro-2-oxo-, (3aS,4S,6aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



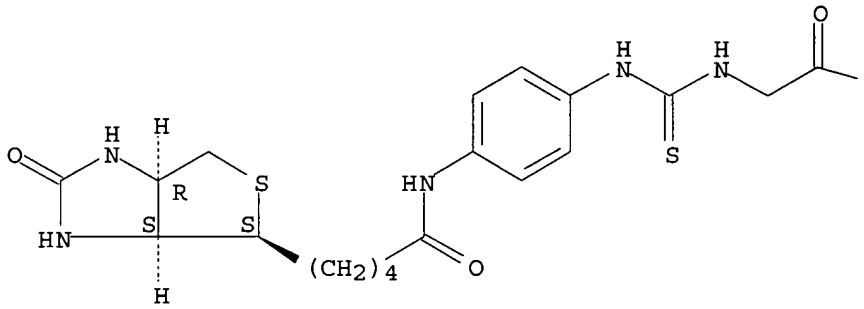
RN 525586-80-5 USPATFULL

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[4-[[[[2-[4-[[4-[[[[[4-(2,5-

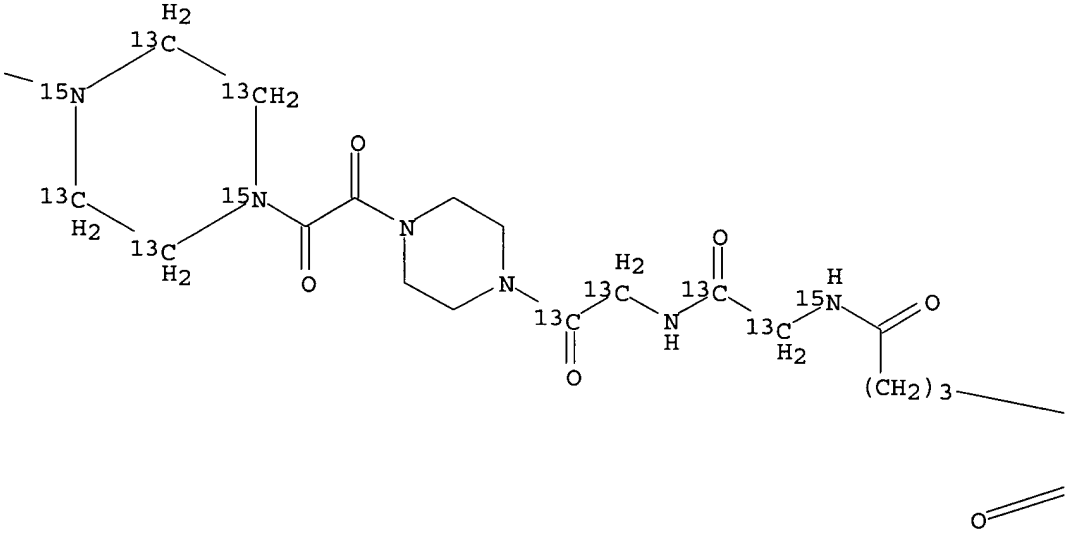
dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl]amino]thioxomethyl]amino]phenyl]hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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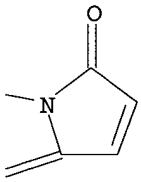
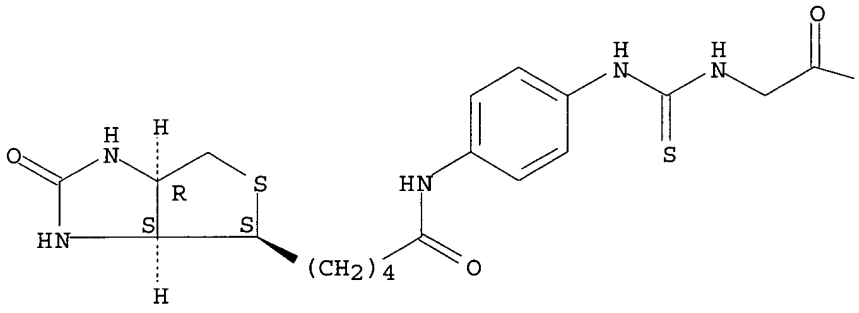


RN 525586-81-6 USPATFULL
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[4-[[[[2-[4-[[4-[[[[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino-15N]acetyl-13C2]amino]acetyl-13C2]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]oxoacetyl]-1-piperazinyl-2,3,5,6-13C4-1,4-15N2]-2-oxoethyl]amino]thioxomethyl]amino]phenyl]hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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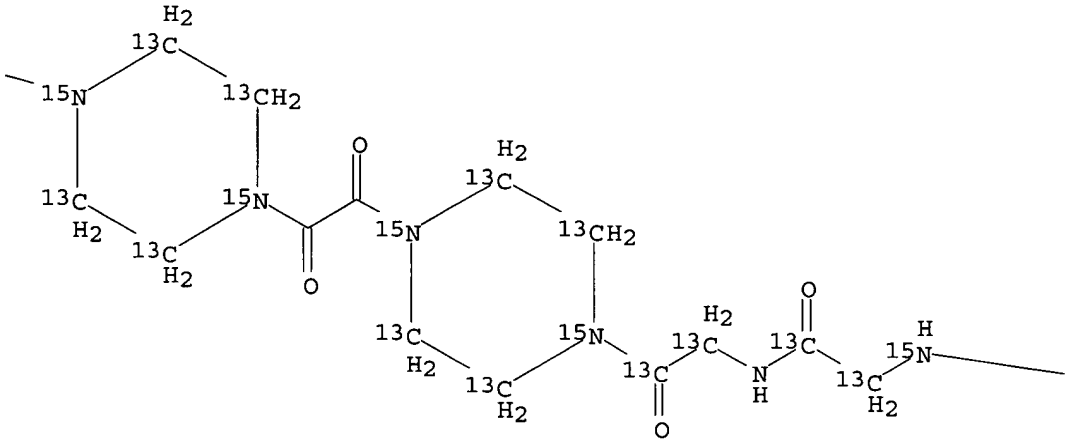

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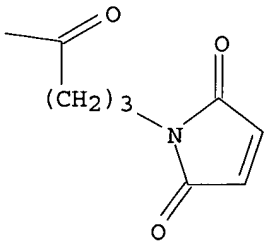


L30 ANSWER 23 OF 25 USPATFULL on STN
ACCESSION NUMBER: 95:34186 USPATFULL
TITLE: Certain 1-methyl-piperidine-4-spiro-4'-(1'-3'-oxazolines) and corresponding -(1',3' thiazolines)
INVENTOR(S): Fisher, Abraham, Holon, Israel
Segall, Yoffi, Ramat Hasharon, Israel
Shirin, Ezra, Tel Aviv, Israel
Karton, Yishai, Ness Ziona, Israel
Meshulam, Haim, Bat Yam, Israel
PATENT ASSIGNEE(S): Israel Institute for Biological Research, Ness Ziona, Israel (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5407938		19950418
APPLICATION INFO.:	US 1993-137690		19931014 (8)

RELATED APPLN. INFO.: Continuation of Ser. No. US 1991-685397, filed on 9 Apr 1991, now abandoned which is a continuation-in-part of Ser. No. US 1990-507708, filed on 10 Apr 1990, now abandoned

DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Rotman, Alan L.
LEGAL REPRESENTATIVE: Darby & Darby
NUMBER OF CLAIMS: 4
EXEMPLARY CLAIM: 1
LINE COUNT: 1356
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

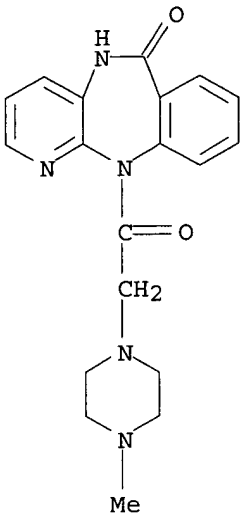
AB The invention relates to compounds (I) for treating diseases of the central and peripheral nervous system, including enantiomers, racemates and acid addition and quaternary salts, ##STR1## wherein Q is selected from two H atoms, (CH.sub.2).sub.m and C(CH.sub.3).sub.2 where m is 1, 2 or 3 and n and p are; each independently 0, 1, 2 or 3, provided that n+p=1-3, and R.sup.0 is H, methyl or OH; the moiety ##STR2## R is selected from H, NH.sub.2, NH-C.sub.1-6 -alkyl, N(C.sub.1-6 -alkyl).sub.2, C.sub.1-6 -alkyl, C.sub.2-6 -alkenyl, C.sub.2-6 -alkynyl, C.sub.3-7 - cycloalkyl, C.sub.1-6 -alkyl substituted by 1-6 halogen atoms, hydroxy- C.sub.1-6 -alkyl, C.sub.1-6 -alkoxy, C.sub.1-6 -alkylthio, C.sub.1-6 -alkoxy-C.sub.1-6 -alkyl, carboxy-C.sub.1-6 -alkyl, (C.sub.1-6 -alkoxy)carbonyl-C.sub.1-6 -alkyl, amino-C.sub.1-6 -alkyl, mono-(C.sub.1-6 -alkyl)amino-C.sub.1-6 -alkyl, di-(C.sub.1-6 -alkyl)amino-C.sub.1-6 -alkyl, 2-oxo-pyrrolidin-1-yl-methyl, aryl, diarylmethylol, and C.sub.1-6 -alkyl substituted by one or two aryl groups; R' is independently selected from the group from which R is selected and C.sub.1-6 -alkanoyl and arylcarbonyl; and aryl denotes unsubstituted phenyl or phenyl substituted by 1-3 substituents selected from halogen, C.sub.1-6 -alkyl, C.sub.1-6 -alkoxy and CF.sub.3, subject to certain provisos.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **124620-97-9**
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)

RN 124620-97-9 USPATFULL

CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



L30 ANSWER 24 OF 25 USPATFULL on STN

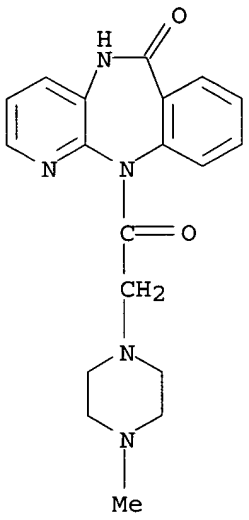
ACCESSION NUMBER:	89:87547 USPATFULL
TITLE:	Oxathiolanes
INVENTOR(S):	Fisher, Abraham, Holon, Israel Karton, Ishai, Ness-Ziona, Israel
PATENT ASSIGNEE(S):	State of Israel, Israel Institute of Biological Research, Israel (non-U.S. government)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4876260		19891024
APPLICATION INFO.:	US 1988-189210		19880502 (7)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1987-114473, filed on 28 Oct 1987, now abandoned		
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Bond, Robert T.		
LEGAL REPRESENTATIVE:	Sheldon & Mak		
NUMBER OF CLAIMS:	43		
EXEMPLARY CLAIM:	1,9		
LINE COUNT:	1306		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention accordingly provides in one aspect, novel spiro-oxathiolane/quinuclidine compounds corresponding with the schematic structural formula (I) ##STR1## and geometrical isomers, enantiomers, diastereoisomers, racemates and acid addition salts thereof, wherein one of Y and Z is 0 and the other is S(.dbd.O).sub.n ; n is 0, 1 or 2; R' and R" are each selected from the group consisting of hydrogen, alkyl, alkenyl, alkynyl, hydroxyalkyl, aminoalkyl, C.sub.3-7 cycloalkyl, aryl, diarylmethylol, and alkyl substituted by at least one aryl group, provided that at least R' and R" is other than hydrogen; and each X is hydrogen, or when Y is 0 and Z is S(.dbd.O).sub.n simultaneously, then each X may also be selected from the group consisting of deuterium and tritium, and provided further that when each X is hydrogen, Y is 0 and Z is S simultaneously, then at least one of R' and R" is selected from the group consisting of alkenyl, alkynyl, cyclopropyl, cyclobutyl, cycloheptyl, hydroxyalkyl and aminoalkyl.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **124620-97-9**
(displacement from rat brain homogenate of, by spiro-oxathiolane/quinuclidine derivs.)
RN 124620-97-9 USPATFULL
CN 6H-Pyrido[2,3-b][1,4]benzodiazepin-6-one, 5,11-dihydro-11-[(4-methyl-1-piperazinyl)acetyl]-, labeled with tritium (9CI) (CA INDEX NAME)



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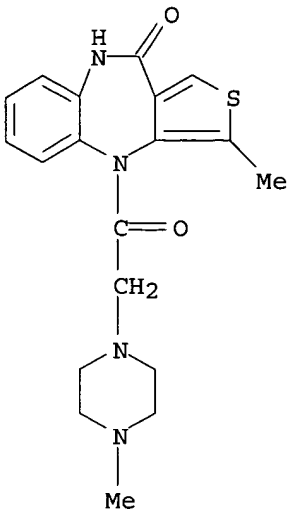
In a multifile environment, a format can only be used if it is valid in at least one of the files. Refer to file specific help messages or the STNGUIDE file for information on formats available in individual files.
REENTER DISPLAY FORMAT FOR ALL FILES (FILEDEFAULT):ide

L30 ANSWER 25 OF 25 CHEMCATS COPYRIGHT 2006 ACS on STN
Accession No. (AN): 2003:3385909 CHEMCATS
Catalog Name (CO): American Radiolabeled Chemicals: Product Listing
Publication Date (PD): 29 Jul 2003
Order Number (ON): ARC1285
Chemical Name (CN): TELENZEPINE, [14C]
CAS Registry No. (RN): **289623-58-1**
Structure :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